NERL/ERD Publications

Technical Information Manager: Janice Sims (706) 355-8011

Jan 1, 1999 - Dec 31, 1999

Presented Published

ABSTRCT/ORAL

Loux, N.T. Issues in assessing low level ionizable contaminant partitioning in soils and sediments. Presented at: Society for Risk Analysis Symposium, Atlanta, GA, December 5-8, 1999. 12/5/1999

Contact: Nicholas T. Loux

Abstract: Solubilization has profound implications for such diverse risk assessment activities as assessing sediment contaminant porewater exposures to benthic fauna, determining half lives of refractory toxicants in natural soils and sediments, and assessing the fate and transport of these compounds in surface and ground waters. The mechanisms governing toxicant partitioning are only partially understood. At high soil/sediment porewater ionizable contaminant concentrations or in the presence of porewater sulfides, dissolved ionic contaminant concentrations can be limited by precipitation reactions with background reactants including hydroxide, bicarbonate, carbonate, sulfate, phosphate and sulfide ligands. In the absence of sulfides and/or at lesser porewater contaminant concentrations, solubility limitations may occur through solid-solution formation by trace toxicants with natural minerals or by adsorption of these compounds on environmental surfaces. The last topic, adsorptive phenomena, is the focus of the present discussion. Many adsorption reactions with trace metals occur through a reaction of the form: Mez+ + >SOH <==> >SOMe(z-1)+ + H + (where Mez+ represents a metal ion of valence z+ and >SOH designates a bound site on an environmental surface; e.g., >SOH can represent an adsorptive site on particulate organic carbon, aluminosilicates, quartz and hydrous oxides of iron, manganese and aluminum). Although it is believed that environmental surfaces display these adsorptive phenomena, limitations exist in our ability to reliably quantify these processes in environmental systems. Specific questions include: 1) can laboratory findings be extended to the field scale, 2) what time period is necessary to assume that equilibrium has occurred, 3) does "irreversible" adsorption occur, 4) are environ-mental adsorptive surfaces "additive" with respect to adsorptive phenomena, and 5) do current surface complexation adsorption paradigms contain assumptions that may be inappropriate for environmental application? These and other questions will be examined.

Burns, L.A. Modelling of agrichemicals in environmental compartments - concepts, problems, and solutions. Presented at: XIVth International Plant Protection Congress, Jerusalem, Israel, July 25-30, 1999. 7/25/1999

Contact: Lawrence A. Burns

Abstract: The potential of plant protection chemicals to migrate away from application sites and expose non-target biota is of continuing interest and concern to regulatory specialists, ecotoxicologists, agriculturalists, and natural resource managers. Regulatory decisions can wait upon neither extensive field experience nor upon complete scientific knowledge of the fate and transport behaviors of chemicals in every relevant physiographic setting. Thus, mathematical and computer-based models are a necessary and critically important part of the risk assessment armamentarium. The more reliable models are solidly based in physical principles (e.g., conservation of mass), algorithmic descriptions of chemical reaction mechanisms, and generalizations from extensive empirical studies of complex environmental behaviors (e.g., sorption to soils and sediments). Given this array of technologies, the completed risk assessment tools must be cast in a form useful to risk assessors, tested for their reliability and accuracy in predicting chemical fate and transport, and their performance quantified in relation to available field experience. In addition, the uncertainties in the predicted quantities must ultimately be characterized either qualitatively, by frequentist methods (e.g., Monte Carlo simulation), or by Bayesian statements of believability. This presentation will review the conceptual underpinnings of exposure analysis, discuss the practical problems encountered in the production of risk assessment tools and their application, enumerate some of the present and future solutions to these problems, and propose research likely to advance the development of more robust decision support systems for agrichemical safety evaluations.

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Kastner, J.R., Santo Domingo, J., Denham, M., Molina, M., and Brigmon, R. Effect of Fenton's reagent on subsurface microbiology and biodegradation capacity. Presented at: 5th International Symposium on In Situ and On-Site Bioremediation, San Diego, CA, April 19-22, 1999. 4/19/1999

Contact: Marirosa Molina

Abstract: Microcosm studies were conducted to determine the effect of Fenton's reagent on subsurface microbiology and biodegradation capacity in a DNAPL (PCE/TCE) contaminated aquifer previously treated with the reagent. Groundwater pH declined from 5 to 2.4 immediately after the treatment, and subsequently rose to a range of 3.4 - 4.0 after 17 months. Groundwater microbial direct counts were approximately two orders of magnitude lower in the treated zone compared to the control after one year. Limited bacterial growth and TCE degradation were detected in the treated zone (pH 3.37 and TCE 5 mg/L) with CH4 and phenol amendments. In contrast, methane addition to groundwater from the up-gradient control well stimulated considerable bacterial growth (pH 4.9 and TCE 0.7 mg/L), indicated by methane consumption, fluorescent antibody analysis, phospholipid based markers, and rDNA probes. TCE degradation was measured in the control microcosms, but only when phenol was added. These results suggest that high TCE concentrations, as well as the lower groundwater pH in the treated zone (i.e., pH 3.37 vs. 4.9) could have inhibited methanotrophic TCE co-metabolism. Bioremediation at the leading edge of plume may be possible, as long the local soil is able to buffer the groundwater pH (e.g.,4.0-4.5). Alternatively, the Fenton's reagent process could be designed to operate at a higher pH (e.g.,4.0-4.5) to minimize detrimental effects, providing an optimal environment to couple advanced oxidation processes with bioremediation technologies.

Wiegert, R.G., Box, E.O., and Lassiter, R.R. The response of animal range to climatic and land-use changes. Presented at: International Congress on Ecosystem Health - Managing for Ecosystem Health, Sacramento, CA, August 15-20, 1999. 8/15/1999

Contact: Ray R. Lassiter

Abstract: The geographic ranges of animal taxa seem much more complex than those of plants, since mobile animals may be constrained by many factors other than readily measurable climatic conditions. These additional factors may include microclimate and availability of particular plant types for food or shelter. Animal range is thus estimated by a combination of climatic envelopes and subsequent "bioenvironment" modeling, in which "bioenvironment" is represented by a model involving the main vegetation characteristics required for food, reproduction and cover. Changes in vegetation have been projected to accompany climatic and land-use changes. As a result, it is expected that animal distributions may also change. Many animals are sensitive to vegetation changes, whether driven by climate or other factors. Potentials for change in animal ranges are evaluated by constructing climate and vegetation envelopes that encompass the functional requirements of selected animal taxa in North America. Projected climatic and land-use changes over the Mid-Atlantic region are used to generate gridded scenarios of potential future conditions in terms of climatic variables used in the climate envelopes. Animal ranges for the change scenarios are estimated by processing the gridded scenario data and constructing maps of projected future distributions. Maps of range changes are utilized to portray the magnitude and location of response, to suggest stresses which may be especially important, and to suggest the degree of vulnerability of existing animal populations to potential future stresses.

Burke, Jr., R.A., Molina, M., Cox, J.E., and Osher, L.J. Use of the composition and stable carbon isotope ratio of microbial fatty acids to study carbon cycling. Presented at: Southeastern Section of the Geological Society of America Symposium, Athens, GA, March 24-26, 1999. 3/24/1999

Contact: Roger A. Burke

Abstract: We use measurements of the concentration and stable carbon isotopic ratio (Gamma 13C) of individual microbial phospholipid fatty acids (PLFAS) in soils and sediments as indicators of live microbial biomass levels and microbial carbon source. For studies of soil organic matter (SOM) cycling, the PLFA Gamma 13C technique is easiest to apply in ecosystems that have undergone a vegetation change (e.g. from C3 to C4 photosynthetic pathway) at known times in the past. For example, in Hawaiian soils we found that conversion of forest to sugar cane cultivation resulted in >65% reduction in total soil PLFA content. In contrast, the total soil PLFA content in a pasture converted from forest long ago (~90 y) was not different from that of the forest soil. PLFA Gamma 13C values strongly reflected the C3 vegetation in the forest sites (-36 to -27 %o), and the C4 vegetation in the pasture site (-19 to -13 %o). PLFA Gamma 13C values from the sugar cane soils (~50 y and 90 y since conversion) were intermediate (-24 to -15 %o), which suggests that either soil microbes have adapted to more recalcitrant, older C3 carbon or that physically-protected labile C3 carbon has been released for microbial use by the greater disturbance of sugar cane cultivation. Application of PLFA Gamma 13C measurements to forest-pasture chronosequence ecosystems should yield valuable information regarding carbon cycling rates by adding a time component to this stable isotope technique.

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Loux, N.T. Charging Contributions to Bound-Site Activity Coefficients with the Entropic Balanced Surface Potential Model. Abstract presented at: American Chemical Society, Anaheim, CA, March 21-24, 1999. — 3/21/1999

Contact: Nicholas T. Loux

Abstract:

Johnston, J.M. A scientific and technological framework for environmental decision making. Presented at: North Atlantic Treaty Organization Advanced Research Workgroup, Sofia, Bulgaria, October 5-9, 1999. — 10/5/1999

Contact: John M. Johnston

Abstract: There are significant scientific and technological challenges to managing natural resources. Data needs are cited as an obvious limitation, but there exist more fundamental scientific issues. What is still needed is a method of comparing management strategies based on projected impacts to ecosystem health. Ecological risk assessment is a field in its infancy, and its focus has been primarily toxic hazards to aquatic endpoints. The expression of sustainable, edible fisheries in an entire estuary as an assessment endpoint, and with greater complexity than a single species or species-by-species approach, is a first challenge. The extension of the scope of a risk assessment to include non-chemical stresses, such as land use change and nitrogen enrichment, is requisite to managing resources given the significance of how these disturbances alter hydrologic balances, habitat characteristics, and even the structure of ecological communities. The separation of intrinsic variability in the status of the fisheries from those variations that result from anthropogenic sources of disturbance is also a challenge that is not trivial. Management alternatives are thus evaluated based on the costs of remediation and related economic and societal issues and the projected changes in resource quality. Ultimately, terrestrial endpoints require attention as well. As an interdisciplinary application of such fields as ecology, biology, environmental management, toxicology, hydrology, and economics, ecological risk assessment requires a much broader, more comprehensive scope and a conceptual framework that synthesizes the contributions of the supporting science and management. These challenges combine with the practical, technological challenges of how to conduct a risk assessment. Central to the goal of performing analyses of various resource management scenarios is the need for a computer-based problem solving environment that automates many of the associated tasks: data gathering and manipulation, integration of statistical, empirical, and mathematical simulation modeling and analysis techniques, and the accommodation of model inter-comparisons within a common framework. Because there are no rules as such for performing an ecological risk assessment, the guidelines that exist as expert knowledge could also be codified and made available within such a framework. It is important to understand that such a framework is much more than simply a collection of assorted tools in a software toolkit. It is the implementation of the science for performing comparative ecological risk. Advances in ecological risk assessment are of a scientific as well as technological nature, and any hoped for state-of-the-art applications of the field must eventually give attention to both areas of need. I present the ongoing development of both a scientific conceptual model for performing comparative risk and a software framework to meet these needs.

Burke, Jr., R.A., Molina, M., and Cox, J.E. Use of stable carbon isotope ratios of fatty acids to evaluate microbial carbon sources in terrestrial environments. Presented at: Soil Science Society of America Annual Meeting, Salt Lake City, UT, November 1- 4, 1999. — 10/31/1999

Contact: Roger A. Burke

Abstract: We use measurements of the concentration and stable carbon isotopic ratio (D 13C) of individual microbial phospholipid fatty acids (PLFAs) in soils as indicators of live microbial biomass levels and microbial carbon source. We found that intensive sugar cane cultivation leads to a reduction in total soil PLFA content (a measure of live microbial biomass) relative to the forest soil. Total soil PLFA content does not appear to be reduced by conversion of forest to pasture or to less intensively managed sugar cane cultivation, however. Data from systems which were converted from tropical forest at different times in the past suggest that the soil microbial community more rapidly and/or completely switches over to use of C4 carbon under pasture than under sugar cane cultivation.

Presented *Published*

Burke, Jr., R.A. Use of the composition and stable carbonIsotope ratio of microbial fatty acids to study carbon cycling. Presented at: Centro de Energia Nuclear na Agricultura (CENA), Sao Paulo, Brazil, September 16, 1999. — 9/16/1999

Contact: Roger A. Burke

Abstract: We use measurements of the concentration and stable carbon isotopic ratio (*13C) of individual microbial phospholipid fatty acids (PLFAs) in soils and sediments as indicators of live microbial biomass levels and microbial carbon source. For studies of soil organic matter (SOM) cycling, the PLFA *13C technique is easiest to apply in ecosystems that have undergone a vegetation change (e.g. from C3 to C4 photosynthetic pathway) at known times in the past. For example, in Hawaiian soils we found that conversion of forest to sugar cane cultivation resulted in >65% reduction in total soil PLFA content. In contrast, the total soil PLFA content in a pasture converted from forest long ago (~90 y) was not different from that of the forest soil. PLFA Delta 13C values strongly reflected the C3 vegetation in the forest sites (-36 to -27 l), and the C4 vegetation in the pasture site (-19 to -13 l). PLFA Delta 13C values from the sugar cane soils (~50 y and 90 y since conversion) were intermediate (-24 to -15 l), which suggests that either soil microbes have adapted to more recalcitrant, older C3 carbon or that physically-protected labile C3 carbon has been released for microbial use by the greater disturbance of sugar cane cultivation. Application of PLFA Delta13C measurements to forest-pasture chronosequence ecosystems should yield valuable information regarding carbon cycling rates by adding a time component to this stable isotope technique.

Rashleigh, B., and Hampson, P. Relation of landscape-scale environmental characteristics to fish assemblages in the upper French Broad River Basin, North Carolina. Presented at: American Fisheries Society Annual Meeting, Charlotte, NC, September 1, 1999. — 9/1/1999

Contact: Brenda Rashleigh

Abstract: Fish assemblages at 16 sites in the upper French Broad river basin in North Carolina were related to environmental characteristics at the landscape scale, the scale at which management activities and decisions are most likely to occur. Indirect gradient analysis and subsequent regression of environmental variables to gradients identified human land-use activities and associated water quality variables as most important in explaining differences in fish assemblages among sites. Agricultural and urban influences on fish assemblages may differ: agricultural influence was represented primarily as a trophic shift from specialized insectivores to omnivores and generalized insectivores, while a secondary urban influence was reflected in a compositional shift from piscivores to sunfish and suckers and an increase in species richness. Results from this study can be used to improve bioassessment techniques in this basin.

Zepp, R.G., Moran, M.A., and Sheldon, W. Changes in spectral and photochemical properties of colored dissolved organic matter in a coastal estuary. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. — 11/14/1999

Contact: Richard G. Zepp

Abstract: Colored dissolved organic matter (CDOM) is the primary determinant of UV penetration and exposure in freshwater and coastal environments. CDOM is photochemically reactive and its photoreactions can lead to reductions in UV absorbance and increased UV exposure in aquatic ecosystems. CDOM also is an important photosensitizer of the production of various reactive oxygen species (singlet molecular oxygen, superoxide, hydrogen peroxide and possibly OH radicals), that influence the oxidizing capacity of surface waters. The fluorescent component of CDOM (FDOM) has been used as an indicator of its concentration and distribution in various aquatic environments. Here we report observations of the changes in photochemical properties, UV-visible and fluorescence spectra and relevant ancillary data along a transect of increasing salinity in the well-mixed estuary of the Satilla River, a high-DOC river located on the Georgia coast.

Zepp, R.G. New approaches to estimating indirect photolysis rates in aquatic environments. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. — 11/14/1999

Contact: Richard G. Zepp

Abstract: Indirect photoreactions in aquatic environments are driven by reactive species, most of which are oxygen centered. Humic substances play an important role in photosensitizing the production of these reactive species, which include singlet molecular oxygen, superoxide ions, hydrogen peroxide, OH radicals and hydrated electrons. In addition, it has been demonstrated recently that photoreactions of humic substances alter their bioavailability, thus influencing microbial activity in surface waters. This paper selectively reviews recent research relevant to estimating indirect photoreactions and will briefly describe the possible role of photochemical-microbial interactions in the fate and transport of compounds in freshwater and

Jan 1, 1999 - Dec 31, 1999

Presented Published

Simon, R., and Weber, E.J. The reductive transformation of perchlorate in a fresh water sediment: laboratory batch studies. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: Eric J. Weber

Abstract: Perchlorate is widely used as a propellant in solid rocket fuel, and has recently been found in ground, surface, and drinking water, in many cases above the interim action level of 18 ppb. Perchlorate is recalcitrant to chemical reduction, however, studies of perchlorate in pure cell cultures and biotechnical systems have demonstrated that microbial reduction does occur. To determine if the reduction of perchlorate would occur under environmentally relevant conditions, laboratory batch experiments using local river sediment and associated site water have been conducted. Perchlorate and its reduction products (chlorate, chlorite, and chloride), as well as redox sensitive species, including nitrate, nitrite, ferrous iron, and sulfate, were measured as a function of time. Perchlorate was reduced to chloride quantitatively in lactate-amended Oconee River (OR) sediment slurries. The addition of lactate was necessary to induce reducing conditions sufficient for the reductive transformation of the perchlorate. Raising the initial concentration of perchlorate from 10 to 60 ppm increased the half-life of the parent compound from 4 to 11 days. At higher aqueous concentrations of perchlorate (100, 1000, and 10,000 ppm), the reduction of perchlorate was not observed, though the microbial activity as indicated by production of carbonate did not change significantly. We speculate that the higher concentrations of perchlorate were toxic to the nitrate-reducing bacteria thought to be responsible for the reduction of the perchlorate. Experimental evidence suggested that nitrate inhibits perchlorate reduction. The lag-phase for the reduction of perchlorate was increased from 2 to 15 days in an OR sediment that had been amended with 60 ppm sodium nitrate, though all of the nitrate had been reduced after four days. Furthermore, the lag-phase for the reduction of perchlorate decreased upon dosing OR sediment with perchlorate after the removal of the indigenous nitrate was observed.

Saleem, Z.A., Ambrose, Jr., R.B., Schwede, D.B., Little, K.L., Guvanasen, D., and Lillys, T.P. Simulating integrated multimedia chemical fate and transport for national risk assessments. Presented at: Society for Risk Analysis Symposium, Atlanta, GA, December 5-8, 1999. 12/5/1999

Contact: Robert B. Ambrose

Abstract: The site-based multimedia, multipathway and multireceptor risk assessment (3MRA) approach is comprised of source, fate and transport, exposure and risk modules. The main interconnected multimedia fate and transport modules are: watershed, air, surface water, vadose zone and saturated zone. These modules predict chemical concentrations for use by the exposure and risk modules. The fate and transport modules calculate the chemical fluxes into downstream media which are linked by sharing data and results files. The source modules produce time series of chemical fluxes as input to these modules. Because of the complex interacting nature of the natural systems being simulated and the implementation of the model in a Monte Carlo framework, the aim of model development was to produce computationally efficient and numerically stable model, while maintaining reasonable accuracy. Numerous innovative enhancements to the legacy media modules were made and several new modules were developed for use in 3MRA. For example, modifications to the air model (ISCST3) included a revised plume depletion algorithm and a modified meteorological sampling approach (SCIM) to reduce computational burden in estimating long-term average chemical deposition values. The Watershed Module simulates the dynamic response of the watershed to atmospheric deposition of a chemical based on a semi-analytical implementation of an enhanced Jury-type fate and transport model, coupled to stormwater runoff and erosion processes. A pseudo-three dimensional module was developed to simulate the fate and transport in aquifers of chemicals and their transformation products with MINTEQ providing the speciation of metals in the subsurface environments. The surface-water module was innovatively enhanced to make it more robust and efficient for simulating waterbody networks at the site. Verifications of the modules and results of application also are discussed.

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Susarla, S., Wolfe, N.L., Garrison, A.W., and McCutcheon, S.C. Perchlorate identification in fertilizers and accumulation in lettuce seedlings. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: Steven C. Mccutcheon

Abstract: Perchlorate has contaminated groundwater, drinking water and soils at several locations in the U.S. The primary source of contamination at sites that have been investigated to date seems to be from industrial and military operations that use Perchlorate as an oxidizing agent. However, recent examination o fseveral fertilizers showed that Perchlorate is present at levels up to 0.84% by weight. Individual experiments conducted with lettuce seedlings over approximately 24 days show that Perchlorate can bioaccumulated by a factor of approximately 350 in the leaves, with little or no transformation. These preliminary results obtained in the absence of soil buffering and competitive ion, suggest that fertilizers could be a source for Perchlorate accumulation in the food chain.

Susarla, S., Wood, G., Wolfe, N.L., and McCutcheon, S.C. Adsorption characteristics of perchlorate in soils. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: Steven C. Mccutcheon

Abstract: Perchlorate(Cl04) is an oxyanion that originates as a contaminant in ground and surface waters from the dissolution of ammonium, potassium, magnesium or sodium salts. Perchlorate is mainly used in solid rocket fuels, explosives, and military batteries. Because of its potential harmful effects perchlorate has recently been added to the EPAs Contaminate Candidate List. The adsorption characteristics of Perchlorate in six different sandy soils was examined in laboratory. The results suggest that Perchlorate sorption was strongly dependent on pH, temperature and organic matter of the soils. The adsorption was maximum around pH 6.5, while temperature had less significant effect. Organic matter present in the soil was primarily responsible for the sorption of Perchlorate. The adsorption data of Perchlorate followed a non-linear Freundlich-type isotherm (S = K C') with n<l and K values between 0.76 and 1.25. Chemisorption is the most probable mechanism for Perchlorate adsorption in these soils.

Williams, T.L., and Collette, T.W. Raman spectral analysis of perchlorate contamination in commonly-used fertilizers. Presented at: Federation of Analytical Chemistry and Spectroscopy Societies Conference, Vancouver, Canada, October 23-29, 1999. 10/23/1999

Contact: Timothy W. Collette

Abstract: Raman spectroscopy (RS) was used for qualitative and quantitative analysis of perchlorate (ClO4-1) in 30+ commonly-used fertilizers. Perchlorate contamination is emerging as an important environmental issue since its discovery in water resources that are widely used for drinking, crop irrigation, and recreation in the western U.S. Perchlorate contamination of substances ingested by humans is a potential health concern because it inhibits iodide uptake by the thyroid, resulting in increased thyroid hormone production.Perchlorate contamination is also found in crops. One potential explanation is that crops bioaccumlate perchlorate from contaminated irrigation water. However, it is also known that perchlorate occurs in Chilean nitrate, which has been widely used in fertilizers. Based on this concern, we and others have analyzed a wide variety of commercial fertilizers, in order to determine the extent of contamination. Perchlorate was typically present at high levels (>500 ppm) in most of these fertilizers.Ion chromatography (IC) with conductivity detection is the recommended method for perchlorate analysis. IC is sensitive (limit of detection of 4 ppb for perchlorate), but exhibits numerous problems for analysis of many environmental samples. They include -- 1) interferences from total dissolve solids (TDS), 2) column fouling, 3) retention time migration with column deterioration and relatively short column life, 4) detector hystersis for gradient elution separations, and 5) qualitative determination based solely on retention time matching. We recently applied RS to the determination of perchlorate in fertilizers and in plant extracts. Most of the problems with IC (or any other chromatographic technique) are not encountered with RS. For example, RS does not exhibit interferences from TDS. If the pH of the sample is below 10.5, then peaks from common fertilizer components (nitrate, sulfate, phosphate, and urea) do not obscure the L1 perchlorate peak at 934 cm-1. In addition, because RS has no upper concentration limits, the time- consuming dilution procedures required of IC are unnecessary for RS. Direct analysis of solid samples is possible. These attributes of RS allow for a short total analysis time to be achieved, and thus RS is better adapted for high-throughput sample analysis. Analysis times for perchlorate determination are ~ 5 min, as compare to ~ 30 min for IC. Finally, qualitative determination by the information-rich vibrational technique of RS is far superior to the retention time matching method. The problems that IC encounters in perchlorate determination are greatly intensified in the more complex matrix of plant extracts. Although the more complex matrix impacts RS as well, the detrimental effect is not nearly as severe. For example, we can readily identify bioaccumlated perchlorate in lettuce extracts that have been exposed to fertilizers and water contaminated with perchlorate.

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Collette, T.W., and Williams, T.L. Optimization of modern dispersive Raman spectrometers for molecular speciation of organics in water. Presented at: Federation of Analytical Chemistry and Spectroscopy Societies Conference, Vancouver, Canada, October 23-29, 1999. 1999. — 10/23/1999

Contact: Timothy W. Collette

Abstract: Pesticides and industrial chemicals are typically complex organic molecules with multiple heteroatoms that can ionize in water. However, models for understanding the behavior of these chemicals in the environment typically assume that they exist exclusively as neutral species -- primarily due to a lack of experimental data on speciation of organics in water. It is clear that this erroneous assumption contributes large uncertainty in chemical exposure assessments when one considers the degree to which chemical behavior (e.g., sorption to soil) differs for different ionization species of the same chemical (e.g., a cation and a neutral). Unfortunately, it has heretofore been prohibitively difficult to study organic chemical speciation in water -- particularly when multiple species exist with the same net ionization charge (such as with zwitterions and tautomers).We have recently developed a method, based on Raman spectroscopy, by which simultaneously occurring site-specific "micro-equilibrium" constants (such as with zwitterions and tautomers) can be determined with confidence. The method involves nonlinear regression modeling of temperature-variant spectral data according to the Gibbs-Helmholtz equation. Success of the method depends on capturing small changes in the observed series of spectra that are due to a systematic change (as a function of temperature) in relative concentration of the species that compose the equilibrium "mixture". In this talk, we will briefly describe the theoretical basis for this method, detail the arduous steps required to obtain an acceptable set of spectra, explore the limitations of assumptions inherent to the method, and make the case that Raman spectroscopy is the ideal tool for this type of environmental investigation.

McCutcheon, S.C., and Pendergast, J. Overview of total maximum daily load (TMDL) problem and supporting model development. Presented at: Appalachian Rivers II Conference, Morgantown, WV, July 27-29, 1999. — 7/27/1999

Contact: Steven C. Mccutcheon

Abstract: Approximately 18,900 impaired water bodies are on the 303(b) state lists required by the Clean Water Act. Of the 300 types of impairments on the 1996 and 1998 lists, 24% involve sediments, suspended solids, or turbidity. Nutrient problems account for 15% of the listings, and pathogens, 14%. The EPA Office of Research and Development (ORD) and the Office of Water are working closely together to develop protocols and models to address TMDL problems in order of frequency of occurrence. The ORD is developing TMDL models under its Ecological Research and Restoration Strategy, and the Office of Water under its pioneering watershed approach. The National Exposure Research Laboratory is developing methods for simpler sediment budgets and more complex sediment routing from watersheds through stratified lakes and estuaries. The EPA Office of Water is working with David Rosgen and interagency partners to develop and test the components method of sediment routing based on extensive experience in stream geomorphology. The range of simple sediment balances, thegeomorphical components analysis, and the more complex multidimensional routing techniques should provide adequate science-based tools to address most sediment TMDLs. Data are being collected for the South Fork of the Broad River in Georgia and with data available from U.S. Agricultural Research Service, the Forest Service, and the U.S. Geological Survey, sufficient testing of new methods and protocols should be possible. By 2004 a case study for nutrient TMDLs is expected that will probably focus on the Neuse River in North Carolina. The ORD expects to focus on pathogens and toxic chemicals during 2005 until 2008. Each component model is being developed using a multimedia modeling context by ORD. In the short-term, the Office of Water has developed the BASINS system to manage data bases and existing water quality models in a manner that can be adapted for each state unless other methods are available.

Presented *Published*

Mack, E.E., Beck, J.W., Mazur, C.S., and Jones, W.J. Environmental characteristics affecting reductive transformation of organic pollutants in anoxic sediments. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: William J. Jones

Abstract: Reductive transformations are important processes for determining the fate of organic pollutants in anoxic environments. These processes are most often microbially mediated by both direct and indirect means. For example, specific bacteria transform organic pollutants directly as co-metabolites or as terminal electron acceptors for the conservation of energy. Alternatively, reduced minerals, generated as products of microbial respiration processes, can serve as reductants for a number of organic pollutants either directly or through a mediator such as natural organic matter. The fates of 3 model compounds, nitrobenzene, 2,4 dichlorophenol, and perchloroethylene were followed in sediment microcosms from four sediments of dfferent physicochemical characteristics. These model compounds were chosen for this study because they contain reducible functional groups with dfferent physicochemical properties. The sediments differed in their ambient concentrations of iron, organic matter, salinity and in situ redox potential. All sediments studied were competent for the reductive transformation of nitrobenzene to aniline but, differences in the competency for transformation of 2,4 dichlorophenol and perchloroethylene were observed. Microbially inhibited controls indicated that nitrobenzene reduction is an example of an indirect microbially mediated reductive transformation. The degree that nitrobenzene reduction was coupled to biotic processes in the different sediments correlated with the presence of microbially produced pools of reduced iron minerals (as characterized by CaCl2, ascorbate and HCl extractable fractions). In contrast, direct microbial transformations of 2,4 dichlorophenol and perchloroethylene were affected by specific physicochemical environmental parameters including redox level, pools of oxidizable organic carbon, and the presence of a competent microbial population.

Ambrose, Jr., R.B., and Burns, L.A. Application of EXAMS as the surface water module in the HWIR multimedia risk assessment system. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/19/1999

Contact: Robert B. Ambrose

Abstract: Multimedia, multipathway risk assessment software has been developed for implementing the Hazardous Waste Identification Rule (HWIR). This regulation is intended to determine whether a waste should be considered hazardous, and confined to Subtitle D facilities, or safely released to Subtitle C disposal. To make this determination for a chemical, a set of multimedia simulations were conducted for 42 chemicals on a representative sample of 201 sites around the country. The Exposure Analysis Modeling System (Exams) was chosen for the surface water module in FRAMES-HWIR. Exams combines chemical loadings, transport, and transformation into a set of differential equations using the law of conservation of mass as an accounting principle. Exams represents water body networks using a series of water column and sediment compartments and a series of physical, chemical, and biological process equations. Exams is linked to FRAMES-HWIR by the ExamsIO module. For each realization in a Monte-Carlo simulation, ExamsIO reads databases describing the site layout, the chemical properties, and the flows and loadings generated by the source, air, land surface, and groundwater modules. This information is used to build an Exams network and an Exams batch input file. ExamsIO then executes Exams and processes its results files for use by other modules in FRAMES-HWIR. Software verification is an important aspect of a development project such as HWIR. Exams and ExamsIO were subjected to several tests, including comparisons with simplified analytical solutions to verify computational setup and accuracy. These efforts have resulted in an accurate, robust surface water module that successfully simulates a wide range of chemicals in a diverse range of water body networks.

Presented *Published*

Wiese, T.E., Garrison, A.W., Nehls, S., and Bishop, T.C. Selective in vitro hormone activity of o,p'-DDT and o,p'-methoxychlor optical Isomers. Presented at: 218th American Chemical Society National Meeting, New Orleans, LA, August 22-26, 1999. 8/22/1999

Contact: Arthur W. Garrison

Abstract: Components and metabolites of the pesticides DDT and Methoxychlor have been described as endocrine disrupting chemicals with estrogen and/or antiandrogen activity. We account the estrogen and antiandrogen activity of the individual enantiomers of o,p'-DDT and o,p'-Methoxychlor. Optically pure samples (separated enantiomers) as well as racemic mixtures were evaluated for steroid receptor binding as well as hormone dependant proliferation and reporter gene activity in mammalian cells. The R(-) enantiomer of o,p'-DDT displayed enhanced estrogen receptor binding activity and was found be significantly more potent in estrogen dependant reporter and proliferation assays than the S(+). While both optical isomers of o,p'-Methoxychlor induced only minimal estrogen activity, an enantiomer selective antiandrogen capacity was observed. This study highlights the importance of resolving the enantiomers of chiral compounds for both endocrine disruptor characterization studies as well as environmental monitoring. Furthermore, we propose that the enantioselectivity of chiral compounds may be utilized to develop optically pure industrial chemicals with minimal endocrine activity.

Bacchus, S.T., Susarla, S., Wolfe, N.L., Harvey, G., and McCutcheon, S.C. Predicting field performance of herbaceous species for phytoremediation of perchlorate. Presented at: 218th American Chemical Society National Meeting, New Orleans, LA, August 22-26, 1999. 8/19/1999

Contact: Steven C. Mccutcheon

Abstract: Results of these short-term experiments coupled with ecological knowledge of the nine herbaceous plant species tested suggest that several species may by successful in on-site remediation of perchlorate. The two wetland species which appear to be most suitable for field experiments for phytoremediation of perchlorate are blue-hyssop and perennial glasswort. Fragrant water-lily appears to be the most promising aquatic species tested for on-site phytoremediation of perchlorate. These three herbaceous plants have the potential to provide effective, economical alternatives for on-site remediation of perchlorate under a variety of conditions.

Bailey, G.W., and Yan, L. Electron transfer mechanism at the solid-liquid interface of phyllosilicates. Presented at: Clays and Clay Minerals Meeting, West Lafayette, IN, June 27-July 1, 1999. 6/27/1999

Contact: George W. Bailey

Abstract: Interfacial electron transfer processes on clay minerals have significant impact in natural environments and geochemical systems. Nitrobenzene was used as molecular probes to study the electron transfer mechanism at the solid-water interfaces of Fe-containing phyllosicates. For this purpose, the oxidation state of structural Fe in Wyoming montmorillonite and ferruginous smectite (SWa-1) were chemically altered. The structural ferric Fe was reduced by sodium dithionite in citrate-bicarbonate (CB) buffer solution under N2 at 70oC, with the excess reactants removed by centrifugation. Both untreated and reduced clay suspensions were reacted with nitrobenzene or benzoic acid water solutions. The UV/Vis spectra of the suspension were collected before and after reacting with the organic probe molecules. Spectral changes in both molecular probes were observed, indicating the presence of new chemical species. These spectral changes were interpreted to mean that electron transfer and free radical formation occurred.

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Simon, R., and Weber, E.J. The reductive transformation of perchlorate in a fresh water sediment: laboratory batch studies. Presented at: 5th International Symposium on In Situ and On-Site Bioremediation, San Diego, CA, April 19-22, 1999. — 4/19/1999

Contact: Eric J. Weber

Abstract: Perchlorate is widely used as a propellant in solid rocket fuel, and has recently been found in ground, surface, and drinking water, in many cases above the interim action level of 18 ppb. Perchlorate is recalcitrant to chemical reduction, however, studies of perchlorate in pure cell cultures and biotechnical systems have demonstrated that microbial reduction does occur. To determine if the reduction of perchlorate would occur under environmentally relevant conditions, laboratory batch experiments using local river sediment and associated site water have been conducted. Perchlorate and its reduction products (chlorate, chlorite, and chloride), as well as redox sensitive species, including nitrate, nitrite, ferrous iron, and sulfate, were measured as a function of time. Perchlorate was reduced to chloride quantitatively in lactate-amended Oconee River (OR) sediment slurries. The addition of lactate was necessary to induce reducing conditions sufficient for the reductive transformation of the perchlorate. Raising the initial concentration of perchlorate from 10 to 60 ppm increased the half-life of the parent compound from 4 to 11 days. At higher aqueous concentrations of perchlorate (100, 1000, and 10,000 ppm), the reduction of perchlorate was not observed, though the microbial activity as indicated by production of carbonate did not change significantly. We speculate that the higher concentrations of perchlorate were toxic to the nitrate-reducing bacteria thought to be responsible for the reduction of the perchlorate. Experimental evidence suggested that nitrate inhibits perchlorate reduction. The lag-phase for the reduction of perchlorate was increased from 2 to 15 days in an OR sediment that had been amended with 60 ppm sodium nitrate, though all of the nitrate had been reduced after four days. Furthermore, the lag-phase for the reduction of perchlorate decreased upon dosing OR sediment with perchlorate after the removal of the indigenous nitrate was observed.

Mack, E.E., Beck, J.W., and Jones, W.J. Biotic and abiotic contributions to reductive transformation of organic pollutants. Presented at: 5th International Symposium on In Situ and On-Site Bioremediation, San Diego, CA, April 19-22, 1999. — 4/19/1999

Contact: William J. Jones

Abstract: The relative contributions of biotic and abiotic reductive transformation reactions were probed in two anoxic freshwater sediments by following the transformation of nitrobenzene, and 2,4 dichlorophenol (compounds with different one electron reduction potentials). The sediments differed in their ambient concentrations of iron, organic matter and in situ redox potential but both sediments were competent for transformation of the test compounds. The transformation of nitrobenzene is known to have both an abiotic and a biotic component. Of the two sediments tested, nitrobenzene reduction in one sediment was found to be predominantly carried out by abiotic pathways while in the other sediment biotic pathways dominated nitrobenzene reduction. Results suggest that the abiotic reduction of nitrobenzene is dependent upon specific pools of reduced iron present in the sediment. In comparison, reductive dechlorination of 2,4 dichlorophenol, a process known to occur via strictly biotic pathways, was limited by availability of organic carbon in one sediment and redox level in the other.

Garrison, A.W. Chiral chemistry of pesticides in the environment with implications for pollution prevention. Presented at: 3rd Annual Green Chemistry and Engineering Conference, Washington, DC, June 29-July 1, 1999. — 6/29/1999

Contact: Arthur W. Garrison

Abstract: Upwards of 25% of pesticides and other toxic pollutants are chiral; that is, they exist as two mirror image species called enantiomers. The enantiomers of a chiral compound have identical physical and abiotic chemical properties, but differ in biological properties such as microbial degradation, uptake and transport across membranes, metabolism rate, and toxicity. Recent research has demonstrated the differences in environmental occurrences, fate and effects of the enantiomers of several chiral pesticides, including alpha-hexachlorocyclohexane, metolachlor, o,p'-DDT, the phenoxypropionic acid herbicides, some organophosphorus compounds, and others. Examples of such research will be given, along with examples of modem analytical techniques for enantiomer separation that are necessary to conduct research on the chirality of pesticides in the environment. Chiral pesticides are almost always manufactured and formulated as their racemic mixtures -- one objective of this research is to make the manufacture and use of single-enantiomer pesticides attractive as a pollution prevention measure, given that the enantiomer that is not active to the target species may have undesirable effects on the environment.

Presented *Published*

Susarla, S., Bacchus, S.T., and McCutcheon, S.C. Perchlorate uptake and transformation in aquatic plants. Presented at: 15th Annual International Conference on Contaminated Sediments, Soils and Water, Amherst, MA, October 12-14, 1999. 10/12/1999

Contact: Steven C. Mccutcheon

Abstract: Ammonium Perchlorate (AP) is produced on a large scale by the chemical industry, for a wide range of applications for example, as a strong oxidizing agent in solid rocket fuel. AP must be washed out of the inventory periodically due to its limited shelf-life,and replaced with a fresh supply. Contamination of groundwater has occurred as the result of these practices. The problem was also compounded by disposal practices during the 1950s through the 1970s, prior to expanded knowledge of the impacts of fuels on ground water and soils. Wastewater generated by industrial use can have AP in the concentration range of grams per liter levels. The large solid rocket motor disposal inventory alone has 55 million pounds of propellant ready for treatment. Over the next 8-10 years this amount is expected to increase to 164 million pounds, which will be targeted for safe disposal. Perchlorate currently is not regulated under the Safe Drinking Water Act, although the California Department of Health Services has established an action level for Perchlorate in drinking water of 18 micrograms per liter. The primary human health concern related to Perchlorate is that it can interfere with the thyroid gland's ability to utilize iodine to produce thyroid hormones, required for normal body metabolism, as well as growth and development. ne majority of data available regarding impacts of Perchlorate on humans is from clinical reports of patients treated with potassium Perchlorate for hyperthyroidism resulting from an autoimmune condition known as graves' disease. Iodine deficiencies in pregnant women are detrimental to fetal development. Interference with the normal function of the thyroid gland, suggests that Perchlorate is an endocrine disrupter. Phytoremediation is the use of plants to cleanse soil and water contaminated with organic or inorganic pollutants. Four vascular plant species were selected for evaluation in these initial experiments. The species of plants included waterweed (Elodea canadensis), parrot-feather (Myriophyllum aquaticum), white water-lily (Nymphaea odorata) and duck meat (Spirodela polyrhiza). Perchlorate was depleted from solution in the presence of parrot-feather and water-lily. Depletion was calculated as a first-order kinetics reaction, with k values (day-1) in sand treatments in the range of 0-0.09 for water-lily. Upper values for parrot-feather was 2. 1. Plant tissues (e.g., roots, stems, leaves) were analyzed for all treatments to identify Perchlorate and its metabolic products. The results showed that Perchlorate, or transformation metabolites (chlorate, chlorite, chloride) were observed in all tissue samples. Results suggested that significant influences on depletion of Perchlorate include: 1) plant species present, 2) concentration of Perchlorate, 3) substrate (sand versus aqueous treatments), 4) the presence or absence of nutrients, and 5) the presence of chloride ions. This study demonstrates that certain plant species withstand exposure to Perchlorate and are also capable of chemically altering a major portion of what is taken up by the plant. If these properties are shared by numerous plant species growing at waste sites, then vascular plants may have a much greater influence on the fate of Perchlorate than has ever been realized. Their potential importance in this regard is further emphasized by recognizing that vascular plants account for the majority of the biomass in terrestrial ecosystems. Thus the results of this study strongly suggest that plants play a major role in governing the fate of Perchlorate.

Wong, C.S., Garrison, A.W., and Richardson, S.D. Enantiomeric Composition of Chiral Haloacetic Acid and Haloacetonitrile Disinfection Byproducts in Drinking Water. Presented at: 217th American Chemical Society National Meeting, Anaheim, CA, March 21-25, 1999. 3/22/1999

Contact: Charles S. Wong

Abstract: Haloacetic acids and haloacetonitriles are well-known chlorine disinfection byproducts (DBPs), formed by the reaction of chlorine with natural organic matter. These compounds are of concern to public health because of their possible toxicological properties. Studies to date on the speciation of these compounds have not examined the enantiomeric composition of bromochloroacetic acid and bromochloroacetonitrile, the two chiral haloacetic DBPs. The enantiomers of these compounds may have different biological and toxicological properties, and may be formed enantioselectively by reaction with chiral centers in humic materials during disinfection. The occurrence and distribution of these chiral DBPs is studied in drinking water samples, and effects of disinfection conditions on the enantiomeric composition of these compounds is discussed.

Shira, B.A., Kenneke, J.F., and Weber, E.J. Reductive Dechlorination of Polyhalogenated Hydrocarbons in Model Systems. 9th Annual Meeting of SETAC-Europe, Leipzig, Germany, May 25-29, 1999. 5/25/1999

Contact: Eric J. Weber

Abstract:

	Presented	Published
Bacchus, S.T., Susarla, S., and McCutcheon, S.C. Application of Vascular Plants for Bioremediation of Perchlorate: Unraveling the Mysteries. 5th International Symposium on In-Situ and On-Site Bioremediation, San Diego, CA, April 19-22, 1999.	4/19/1999	
Contact: Steven C. Mccutcheon		
Abstract:		
Kenneke, J.F., and McCutcheon, S.C. A Long-Term Laboratory and Field Investigation on the Degradation of PCE with Zero-Valent Iron. Geological Society of America, Southeastern Section Meeting, Athens, GA, March 25-26, 1999.	3/25/1999	
Contact: John F. Kenneke		
Abstract:		
Bacchus, S.T., Susarla, S., and McCutcheon, S.C. Advantages of a Multidisciplinary Approach to In Situ Phytoremediation. Georgia Water Resources Conference, Athens, GA, March 29-31, 1999.	3/29/1999	
Contact: Steven C. Mccutcheon		
Abstract:		
Simon, R., Colon, D., and Weber, E.J. Effect of DOM and Redox Zonation on the Reductive Transformation of Nitroaromatics: Batch and Laboratory Column Studies. 9th Annual Meeting of SETAC-Europe, Leipzig, Germany, May 25-29, 1999.	5/25/1999	
Contact: Eric J. Weber		
Abstract:		
Tsiros, I.X., Ambrose, Jr., R.B., and Chronopoulou-Sereli, A. Air-Vegetation-Soil Partitioning of Toxic Chemicals in Environmental Simulation Modeling. 6th International Conference on Environmental Science and Technology, Samos, Greece, Aug. 31 - Sept. 2, 1999.	8/31/1999	
Contact: Robert B. Ambrose		
Abstract:		
Wiese, T.E., and Garrison, A.W. Selective Estrogen Activity of o,p'-DDT and o,p'-DDD Enantiomers. Annual Meeting of the Society of Toxicology, New Orleans, LA, March 14-18,	3/14/1999	
Contact: Arthur W. Garrison		
Abstract:		
Gao, J., Garrison, A.W., Hoehamer, C., and Wolfe, N.L. Biotransformation of Organophosphorus Pesticides and DDT Using Axenic Plant Tissue Cultures. 5th International Symposium on In Situ and On-Site Bioremediation, San Diego, CA, April 19-22, 1999.	4/19/1999	
Contact: Arthur W. Garrison		
Abstract:		

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Tsiros, I.X., Ambrose, Jr., R.B., and Laniak, G.F. Simulation models for environmental multimedia analysis of toxic chemicals. Presented at: 3rd International Conference on Environmental Technology, Thessaloniki, Greece, June 3-6, 1999. — 6/3/1999

Contact: Robert B. Ambrose

Abstract: Multimedia understanding of pollutant behavior in the environment is of particular concern for chemicals that are toxic and are subject to accumulation in the environmental media (air, soil, water, vegetation) where biota and human exposure is significant. Multimedia simulation modeling involves the simultaneous tracking of environmental stressors from a source through air, water, and soil to locations where human populations or ecological components may be exposed. By estimating realistic and technically valid distribution of emissions under a variety of scenarios, multimedia-based simulation models can be useful screening-level tools that can help both regulatory agencies and industry develop the best operating and control strategies to reduce risks. The purpose of this paper is to review the several approaches to multimedia modeling technology and to evaluate selected multimedia simulation models. First, a general comparison of the available multimedia modeling approaches is presented. Detailed evaluations of model components and capabilities are also presented for selected models. Significant differences in model capabilities as well as useful features of each of the models are identified; models differ with respect to environmental processes included and the mathematical formulation and assumptions related to the implementation of solutions. In addition, simulations were performed to investigate formulations and functions of the model by benchmarking analysis. Model capabilities and limitations of the state-of-the-art environmental multimedia modeling technology are also discussed from a user's point of view.

Wong, C.S., Garrison, A.W., and Richardson, S.D. Enantiomeric Composition of Chiral Haloacetic Acid and Haloacetonitrile Disinfection By-products in Drinking Water. American Chemical Society, Anaheim, CA, March 21-24, 1999. — 3/21/1999

Contact: Charles S. Wong

Abstract:

Wong, C.S., and Garrison, A.W. Enantioselectivity in the Aerobic and Anaerobic Biotransformation of Chiral Polychlorinated Biphenyl Atropisomers. American Chemical Society, Anaheim, CA, March 21-24, 1999. — 3/21/1999

Contact: Charles S. Wong

Abstract:

Lewis, D.L., and Garrison, A.W. Global effects of various soil treatments on transformations of chiral pesticides. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. — 11/14/1999

Contact: Arthur W. Garrison

Abstract: Many pesticides and other organic pollutants are chiral, and their enantiomers exhibit differences in biological properties, including rates of microbial degradation. We have measured by chiral GC and capillary electrophoresis the enantioselectivity of biodegradation of three pesticides --ruelene (an organophosphorus insecticide) and dichlorprop and methyl dichlorprop (phenoxyacid herbicides) -- as probes of the microbial population character of disturbed/treated and control soil samples from field plots located in Brazil, North America and Norway. We found that each type of disturbance (deforestation) and treatment (nutrient amendments and warming at 5oC above ambient temperature to simulate global warming) shifted enantiomer specificity of the soil microbial populations for biodegradaion of the pesticides. For example, soil microorganisms in most forest samples from Brazil removed the (+) enantiomer of dichlorprop, the active form of the herbicide. By comparison, those in pasture samples almost exclusively preferred the (-) enantiomer. Consequently, in the tropical forests herbicide concentrations determined by conventional achiral methods largely represented the presence of the inactive form. Nutrient enrichments shifted enantioselectivity for the herbicide ester strongly toward preferentially removing the (-) enantiomer, thus potentially increasing the phytotoxicity of herbicide residues. These results show that historical correlations between pollutant exposure and health effects or environmental damage may be unreliable in many cases where chirality has been neglected. Any valid adverse effects of these pollutants could either be abated or exacerbated by future environmental change affecting enantioselectivity of biodegradation processes.

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Wong, C.S., Garrison, A.W., Foreman, W.T., Capel, P.D., and Nowell, L.H. Enantiomeric occurrence and distribution of chiral organochlorine compounds in U.S. river sediment and biota. Presented at: 218th American Chemical Society National Meeting, New Orleans, LA, August 22-26, 1999. — 8/22/1999

Contact: Charles S. Wong

Abstract: River sediment and biota (fish, bivalves) from throughout the continental U.S. were analyzed for chiral organochlorine compounds (o,p'-DDT and DDD, some chlordane compounds, PCB atropisomers) to assess spatial trends in environmental chirality. Chiral PCB enantiomers were racemic in most sediment, but were nonracemic at sites heavily impacted by PCBs and subject to reductive dechlorination. Pesticide enantiomers were present in nonracemic quantities in both media, suggesting enantioselective processing; however, enantiomeric ratios of PCBs and pesticides were significantly different between sediment and biota taken at the same site and time, suggesting enantioselective processes in biota (uptake, metabolism, depuration) not present in sediment. Enantioselectivity was reversed between fish and bivalves for some compounds.

Wolfe, N.L., Collette, T.W., Garrison, A.W., Susarla, S., and Teng, Q. Alternative techniques for measurement of perchlorate in fertilizer and environmental samples. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. — 11/14/1999

Contact: Nelson L. Wolfe

Abstract: The Perchlorate anion has been implicated as a potentially serious environmental pollutant, being found in drinking water and irrigated crops. Commercial fertilizers have recently been shown to contain high levels of Perchlorate impurities and thus be potentially important sources of the pollutant. Ion chromatography (IC) with conductivity detection is the established technique for Perchlorate analysis in environmental samples. In investigating the occurrences of perchlorate in various fertilizers, however, it became necessary to develop techniques for confirmation of Perchlorate and, if possible, for improved routine quantitative analysis. Thus, we have investigated the applications of 3 widely varying analytical technologies to this problem: 1) capillary electrophoresis (CE), 2) Raman spectroscopy (RS), and 3) NMR spectroscopy. In each case, trial samples consisted of simple filtered aqueous extracts, diluted if necessary, of 8 solid commercial fertilizers of varying composition. CE involved a coated column to reduce the electroosmotic flow, using reversed polarity and indirect UV detection with pyromellitic acid as visualization reagent. Perchlorate, chlorate, chlorite, and chloride were separated, detected and quantified by this method. RS using 785nm diode laser excitation and a fiber optic probe coupled with a charge-coupled-device detector provided an unambiguous fingerprint for all these anions except chloride; the Perchlorate spectrum from the fertilizer solutions could be obtained directly through the glass sample vial. NMR of the 35Cl nucleus resulted in a single sharp peak specific for the Perchlorate species. Using each of these techniques, the presence of the Perchlorate anion was confirmed in each fertilizer sample. Further research is underway to determine detection limits and other analytical parameters for each of the techniques when applied to the measurement of anionic chlorine species in various fertilizers.

Garrison, A.W. An overview of chiral chemistry in the environment. Presented at: 218th American Chemical Society National Meeting, New Orleans, LA, August 22-26, 1999. — 8/22/1999

Contact: Arthur W. Garrison

Abstract: Upwards of 25% of pesticides and other toxic organic pollutants are chiral; that is, they exist as two mirror image species called enantiomers. The enantiomers of a chiral compound have identical physical and abiotic chemical properties, but usually differ in biological properties such as microbial degradation, uptake and transport across membranes, metabolism rate, and toxicity. Ove the past decade, a few analytical and environmental chemists have begun to investigate this enantioselectivity phenomenon in environmental samples, accumulating data that provide a more accurate assessment of pesticide and PCB transport, exposure and effects. This overview will give historical examples of enantioselectivity in the degradation rates and occurrences of the enationmers of chiral pollutants in various environmental compartments and biota. In addition, recent work from the author's lab will be summarized to illustrate analytical separations of enantiomers as well as enantioselectivity in the environment.

Presented *Published*

Garrison, A.W., Wong, C.S., Pakdeesusuk, U., Lee, C.M., Coates, J.T., and Elzerman, A.W. Enantiomeric ratios of chiral PCB atropisomers in radiodated sediment cores. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: Arthur W. Garrison

Abstract: Enantiomeric ratios (ERs)) of chiral polychlorinated biphenyl (PCB) atropisomers were quantified in radiodated sediment cores of Lake Hartwell SC, a reservoir heavily impacted by PCBS, to study spatial and temporal changes in chirality. A chiral analysis of cores showed accumulation of PCBs with depth in sediments consistent with the use history and contamination in Lake Hartwell, suggesting from changes in congener patterns and increasing concentration of ortho-only congeners, end-products of meta- and para-dechlorination, that reductive dechlorination was occurring in situ in sediments. Chiral analysis showed enantioselective occurrence of some PCB atropisomers with depth, indicating that the reductive dechlorination processes in Lake Hartwell are stereospecific, and suggesting that changes in ER with depth can be a chronological tracer in sediments.

Long, J.M., Karickhoff, S.W., Weber, E.J., and Jones, W.J. SPARC generated chemical properties database for use in national risk assessments. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: Jesse M. Long

Abstract: The SPARC (Sparc Performs Automated Reasoning in Chemistry) Model was used to provide temperature dependent algorithms used to estimate chemical properties for approximately 200 chemicals of interest to the promulgation of the Hazardous Waste Identification Rule (HWIR) . Properties included acid/base ionization, Henry?s Law Constant, Solubility, KOW, molar volume, gas diffusion, density, sorption and water diffusivity.. For consistency and technical balance, the temperature dependence of all physical/chemical process parameters was represented as log-linear functions of 1/T (i.e., linear functions on a free energy basis). For chemicals that ionize, the physical properties (at a given pH and T) were weighted over all

Simon, R., and Weber, E.J. The reductive transformation of perchlorate in a fresh water sediment: laboratory batch studies.. Presented at: 218th American Chemical Society National Meeting, New Orleans, LA, August 22-26, 1999. 8/20/1999

Contact: Eric J. Weber

Abstract: Perchlorate is widely used as a propellant in solid rocket fuel, and has recently been found in ground, surface, and drinking water, in many cases above the interim action level of 18 ppb. Perchlorate is recalcitrant to chemical reduction, however, studies of perchlorate in pure cell cultures and biotechnical systems have demonstrated that microbial reduction does occur. To determine if the reduction of perchlorate would occur under environmentally relevant conditions, laboratory batch experiments using local river sediment and associated site water have been conducted. Perchlorate and its reduction products (chlorate, chlorite, and chloride), as well as redox sensitive species, including nitrate, nitrite, ferrous iron, and sulfate, were measured as a function of time. Perchlorate was reduced to chloride quantitatively in lactate-amended Oconee River (OR) sediment slurries. The addition of lactate was necessary to induce reducing conditions sufficient for the reductive transformation of the perchlorate. Raising the initial concentration of perchlorate from 10 to 60 ppm increased the half-life of the parent compound from 4 to 11 days. At higher aqueous concentrations of perchlorate (100, 1000, and 10,000 ppm), the reduction of perchlorate was not observed, though the microbial activity as indicated by production of carbonate did not change significantly. We speculate that the higher concentrations of perchlorate were toxic to the nitrate-reducing bacteria thought to be responsible for the reduction of the perchlorate. Experimental evidence suggested that nitrate inhibits perchlorate reduction. The lag-phase for the reduction of perchlorate was increased from 2 to 15 days in an OR sediment that had been amended with 60 ppm sodium nitrate, though all of the nitrate had been reduced after four days. Furthermore, the lag-phase for the reduction of perchlorate decreased upon dosing OR sediment with perchlorate after the removal of the indigenous nitrate was observed.

Presented *Published*

Yan, L., and Bailey, G.W. Using molecular probes to study interfacial redox reaction at Fe-bearing smectites. Presented at: Soil Science Society of America Annual Meeting, Salt Lake City, UT, November 1- 4, 1999. 10/31/1999

Contact: George W. Bailey

Abstract: The interfacial electron transfer of clay-water systems has a wide range of significance in geochemical and biogeochernical environments. However the mechanism of interfacial electron transport is poorly understood. The electron transfer mechanism at the solid-water interfaces of Fe-containing smectites was investigated. In this study nitrobenzene and benzoic acid were used as molecular probes. Both untreated and reduced smectite suspensions were reacted with the probe water solutions. At the end of reaction the solution phases were separated by centrifuge, and were analyzed by HPLC with photo diode array UV detector. It was found that, only in the reduced smectite suspensions, nitrobenzene was reduced and transformed into aniline, and benzoic acid was transformed into hydroxybenzoic acids. These results were interpreted to mean that electron transfer and free radical formation occurred.

Lewis Hutchinson, S., Susarla, S., Wolfe, N.L., and McCutcheon, S.C. Perchlorate accumulation from fertilizer in leafy vegetation. Presented at: 218th American Chemical Society National Meeting, New Orleans, LA, August 22-26, 1999. 8/19/1999

Contact: Stacy L. Lewis

Abstract: Perchlorate contaminated water and soil has been identified in many areas of the United States. Previous studies indicated that the primary source of contamination was from industry and military operations that use perchlorate as an oxidzing agent. However, recent studies have found significant quantities of perchlorate in commercial fertilizers, which may be an additional source of perchlorate in the environment. Current studies on vegetation uptake of perchlorate from fertilizer show that leafy garden crops, lettuce (Lactuca sativa) and mustard (Brassica alba), accumulate perchlorate and its transformation products in their leaves, stems, and roots. Final results have not been tabulated and additional experimental work is needed to confirm preliminary findings.

Jan 1, 1999 - Dec 31, 1999

Presented Published

Chen, Y.D., McCutcheon, S.C., Nutter, W.L., and Carousel, R.F. Hydrologic and stream temperature modeling for anadromous fish habitat restoration in a wildland watershed. Presented at: American Water Resources Association Annual Summer Specialty Conference on Wildland Hydrology, Bozeman, MT, June 30-July 2, 1999. 6/30/1999

Contact: Steven C. Mccutcheon

Abstract: Reduction or removal of streamside vegetation by logging and grazing can alter stream temperatures by reducing riparian shading. In the Pacific Northwest of the United States and other parts of the world, elevated stream temperatures in summer are a major fish habitat degradation problem that affects coldwater species such as salmon and trout. For example, the lethal temperature for Chinook Salmon is approximately 26oC, and sublethal effects on juveniles can occur at significantly lower temperatures. Projects to restore riparian forest cover are often intended to reestablish shading and reduce stream temperatures to levels that can support coldwater communities. To provide guidance for riparian vegetation restoration activities, comprehensive and dynamic information about stream temperature regimes can be cost-effectively generated by watershed-scale, continuous stream temperature modeling. The Hydrologic Simulation Program - FORTRAN (HSPF), a major watershed modeling tool developed and supported by US Environmental Protection Agency (USEPA) and US Geological Survey (USGS), together with its supporting data management programs and expert system software for model calibration, form a comprehensive watershed hydrology and water quality modeling system that may be used to conduct hydrologic/hydraulic and stream temperature simulations. Solar radiation is the primary source of energy for stream heating. To simulate stream temperature dynamics, hillslope topographic shade angles and geometric dimensions of riparian vegetation buffers (if any) must be used for estimating the amount of solar energy that actually reaches the stream surface. Because of the limitation of modeling technology and the lack of basin-wide riparian shading characteristics, watershed-scale and continuous-based simulation of stream temperature in forest basins was not possible in the past. Traditional field observations using solar pathfinder and other equipment can only estimate a few averaged parameters of riparian shading characteristics as input to reach-scale stream temperature models. With the advances in remote sensing and GIS technologies, extensive data representing the detailed characteristics of stream channel, hillslope topography, and riparian vegetation buffers can be effectively created and processed. In order to use the GIS-derived riparian shading characteristics for watershed-scale stream temperature modeling, a computer model called SHADE was developed for computing the shading dynamics and thus the effective solar energy for stream heating. The SHADE-generated radiation data are used by HSPF to simulate hourly stream temperatures that can be used to target critical stream reaches for fish habitat restoration and to evaluate the effectiveness of replanting riparian vegetation. The SHADE-HSPF modeling system was calibrated, and then validated for the Upper Grande Ronde (UGR) watershed in northeast Oregon, USA.The module section HTRCH in HSPF is a one-dimensional code for simulating water temperature of each reach of a stream network. In HTRCH, the energy budget analysis technique is employed to determine the net heat exchange for simulating stream temperature dynamics. However, HTRCH did not originally have the capability to provide a realistic estimate of the amount of incoming solar radiation that actually enters stream water, due to the lack of adequate algorithms for vegetation and topographic shading computations. Therefore, SHADE was developed for dynamically estimating the contribution of riparian vegetation buffers and topography to stream surface shade. SHADE, together with, HSPF and its four supporting programs (ANNIE, METCMP, SWSTAT, and HSPEXP) form a watershed hydrology and stream temperature modeling system. In the SHADE-HSPF modeling system, GIS-derived topographic and vegetation shading characteristics are used by SHADE for computing the width of shade which is compared against the stream surface width (TWID, simulated by the hydraulic module section HYDR in HSPF) for estimating the percentage of shaded stream surface at each time interval. By doing so, SHADE computes the amount of effective solar radiation for stream heating, as indicated by the input of unadjusted radiation and the output of adjusted radiation for stream temperature simulation by HTRCH in HSPF. SHADE also generates solar radiation factor (SRF, the ratio of radiation effective for stream heating divided by the incoming radiation before any reduction by shading) values that can be used to characterize the dynamic shading conditions.The SHADE-HSPF modeling system was applied to simulate the watershed hydrology and stream temperatures in the UGR watershed. Simulation results confirmed the accuracy and robustness of the modeling system. To identify the possible causes for reducing the high summer stream temperatures, the impacts of hydroclimatic shifts and hypothetical riparian vegetation buffers were evaluated. Simulations demonstrated that natural weather cycles of ?10% or ?20% in air temperature, solar radiation, and precipitation can not sufficiently moderate the stream temperature regimes to insure the survival and reproduction of salmon. Therefore, riparian vegetation is the only critical factor that can be managed to alleviate significantly the lethal and sub-lethal stream tempera-tures. Stream temperature forecasts for restored riparian buffers demonstrate that 44 out of 51 reaches in the watershed could achieve a no-effect standard that includes a maximum summer temperature of 16oC and average 7-day maximum temperature of 14.5oC. Downstream reaches (the 5th order) on the mainstem Grande Ronde River are too wide to be sufficiently shaded by restored buffers to meet this standard. The creation of thermal refugia or other management practices, inaddition to riparian restoration, may be required if studies of the threatened salmon species show that the lower mainstem is the critical habitat.Simulated maximum values of stream temperature, on which the riparian restoration forecasts are based, are accurate to 2.6 to 3.0oC. Hourly simulations have approximately the same

accuracy and precision. The phase, diurnal fluctuations, and day-to-day trends in stream temperature simulations are very good, confirming the validity of shading computations and the observed air temperatures. Occasionally, the model conservatively oversimulated, especially in localized areas where cool ground-water in-flow may dominate. The difference in the spatial resolution between the reach-averaged simulations and the point measurements of stream temperature, together with other data uncertainties such as the limited precision and accuracy of riparian shading characteristics and the lack of extensive channel morphological data, caused some systematic simulation errors for over a third of the 27 calibration sites (11 sites in 1991 and 12 sites in 1992).The application study demonstrated the validity and usefulness of the SHADE-HSPF modeling system. With the SHADE-generated solar radiation data, HSPF can accurately simulate reach-averaged stream temperatures at the watershed scale by accounting for the riparian shading characteristics and the thermal impacts of basin-wide land cover on the runoff temperatures. Compared to the 8 to 10oC violations of the temperature standards under the present riparian vegetation conditions in the Upper Grande

Lewis Hutchinson, S., Susarla, S., and McCutcheon, S.C. Perchlorate crop interactions via contaminated irrigation water. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: Stacy L. Lewis

Abstract: Perchlorate has contaminated water and sods at several locations in the United States. Perchlorate is water soluble, exceedingly mobile in aqueous systems, and can persist for many decades under typical ground- and surface water conditions. Perchlorate is of concern because of uncertainties about toxicity and health effects from low levels in drinking water, the impact on ecosystems, and possible indirect exposure pathways for humans from agricultural and other activities. To determine the impact of irrigating crops with contaminated water, a greenhouse study was conducted using tomato and green pepper plants. Both surface and subsurface irrigation application techniques were simulated with 3 replicates of each treatment. Four Perchlorate concentrations, 0.02mg/L, 0.2 mg/L, 2.0 mg/L, and 20.0 mg/L, and a zero control, were applied to the vegetation. At maturity, the plant was separated by leaves, stems, roots, and fruit. Plant tissue was analyzed for Perchlorate uptake, accumulation, and transformation products.

Ellington, J.J., Evans, J.J., and Cook, S.C. Enzyme degradation of chiral organic phosphorus insecticides. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/14/1999

Contact: James J. Ellington

Abstract: Chiral organic phosphorus pesticides (OPs) are expected to be biologically degraded enantioselectively by endogenous enzymes. Various chiral Ops were treated with the enzyme phosphotriesterase (PTE) obtained from partially purified extracts of Escherichia coli strain DH-5- carrying a cloned opd gene from Flavohacterium. The enzymatic degradation of the OP enantiomers was followed by HPLC using a Chiraicel OJ chiral column. Initial results, using the OP Crotoxyphos, indicated that each enantiomer of Crotoxyphos degraded at a different rate. UV-Vis spectrometry was used to determine the overall rate constant for the racemic

Ellington, J.J., and Evans, J.J. Occurrence of perchlorate anion in plant organs: method development and results of analysis of selected plants. Presented at: 20th Annual Society of Environmental Toxicology and Chemistry Meeting, Philadelphia, PA, November 14-18, 1999. 11/15/1999

Contact: James J. Ellington

Abstract: Perchlorate has recently been detected in ground and surface waters in several western states. Perchlorate is a mobile and persistent oxy anion of chlorine. Ongoing laboratory studies demonstrated that perchlorate is transported from perchlorate fortified soil to the plant and accumulated in the plant tissues and organs. A standardized method for the analysis of perchlorate in plants was developed, based on dry weight, and applied to the analysis of contaminated plants.

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Frick, W.E., Phelps, H., Sigleo, A.C., and Barber, M.C. Naturalist's application of a promising turbulence model. Presented at: 80th Western Society of Naturalists Annual Meeting, Monterey, CA, December 26-30, 1999. 12/26/1999

Contact: Walter E. Frick

Abstract: Turbulence has infinite applications to the biological sciences, affecting distributions, transport, feeding, mating, and other biological processes. The topic is like the universe for which five successive magnefications are required to finally focus on a topic that can be grasped by the individual researcher, such as the effect of turbulence on benthic organisms. Even at this level a myriad of questions arise: All clam syphons are fimbriated, with little projections all around, sometimes rather brightly colored. Surely that must dissipate the flow and decrease the turbulence. How much? The entrance syphons are always shorter and broader than the exit. How can they disturb the benthic water boundary layer sufficiently to guarantee fresh water (and access to food)? Why are the entrance siphons of filter-feeding clams so much different in construction than those of clams who use them to primarily suck up food off the neighboring bottom (thinner and more muscular). Yet, extant turbulence models tend to be advanced concepts relegated to esoteric physical and mathematical disciplines, involving boundary layers, the Navier-Stokes non-linear equations, and mathematical decompositions, accessible primarily to programmers of supercomputers. An innovative theory brings an understanding of the important properties and consequences of turbulence to the naturalist. The theory helps to explain many phenomena important to their disciplines. For example, it makes apparent the formation of turbulent boundary layers around organisms and helps predict the concomitant forces in qualitative terms. It helps to explain the dissipation of topologically generated energetic jets, and the effect on mixing and distribution of suspended materials. And, it offers an explanation for the separation of suspended materials in turbulent flows.

Hayter, E.J. Prediction of contaminated sediment transport in the Maurice River-Union Lake, New Jersey, USA. Presented at: United Nations Educational, Scientific and Educational Organization Meeting "A Sediment Transport Model of the Inner Channels of Venice", Venice, Italy, June 28-29, 1999. 6/28/1999

Contact: Earl J. Hayter

Abstract: This paper describes a sediment and contaminant transport model and its application to the Maurice River-Union Lake system in southern New Jersey, USA for the purpose of characterizing and forecasting sediment and arsenic distributions before and after proposed dredging activities. The model, HSCTM-2D, is a two-dimensional, depth-averaged finite element model capable of simulating the hydraulics of both steady and unsteady surface water flows, cohesive and cohesionless sediment transport, and the transport and fates of inorganic contaminants, specifically metals and metalloids. Interactions between dissolved (i.e., desorbed) and participate (i.e., adsorbed) contaminants and sediments are accounted for by simulating the processes of adsorption and desorption of contaminants to and from sediments, respectively. Four model simulations yielded flushing times ranging from 15 years for the "no action" scenario to 4 years for dredging of contaminant bed sediments in the Maurice River and Union Lake.

Frick, W.E. Individual turbulent cell interaction: basis for boundary layer establishment. Presented at: Estuarine Research Federation 15th Biennial Conference, New Orleans, LA, September 25-30, 1999. 9/25/1999

Contact: Walter E. Frick

Abstract: Boundary layers are important in determining the forces on objects in flowing fluids, mixing characteristics, and other phenomena. For example, benthic boundary layers are frequently active resuspension layers that determine bottom turbidity and transniissivity. Traditionally, boundary layer theory has been based on the assumption of incompressible flow, and are often treated by random mathematical methods. However, recently it was shown that turbulent flow is inherently compressible flow and that turbulence is comprised of short-lived, physically-definable cells. This theory suggests that pressure disturbances caused by turbulent density fluctuations can vary considerably from those derived from our understanding of the Bernoulli effect for incompressible flow. This work builds on the new theory for turbulence to synthesize bursts of turbulent flow in an attempt to define boundary layers in shear flow.

Presented *Published*

Richardson, S.D. Identification of new drinking water disinfection by-products from ozone, chlorine dioxide, chloramine, and chlorine. Presented at: 7th International Conference of the Israel Society for Ecology and Environmental Quality, Tel Aviv, Israel, June 13-18, 1999. — 6/13/1999

Contact: Susan D. Richardson

Abstract: Due to concern over the potential adverse health effects of trihalomethanes (THMs) and other chlorinated by-products in chlorinated drinking water, alternative disinfection methods are being explored. Ozone, chlorine dioxide, and chloramine are currently popular alternatives to chlorine, as they kill microorganisms effectively, but do not produce appreciable levels of THMs, which are regulated by many countries. Although these alternative disinfectants are widely used, there is little information on the DBPs they produce. Are they safer or more harmful than those formed by chlorine? To answer this question and to ultimately determine if there are harmful DBPs that should be minimized, our laboratory has been carrying out comprehensive studies aimed at identifying all detectable disinfection by-products (DBPs) from these alternative disinfectants. To identify these new DBPs, we are using GC/MS (EI and CI, low and high resolution), GC/IR, and LC/MS. Using these techniques, we have identified many DBPs from ozone, chlorine dioxide, chloramine, and chlorine, many of which have never been reported previously. A comparison of DBPs identified to-date will be presented. Also, we have recently begun a project to identify DBPs from Israel drinking water. Preliminary results of that research will be presented.

Chen, P.H., Richardson, S.D., Thruston, Jr., A.D., and Krasner, S.W. Investigations into the GC/MS decomposition of tribromonitromethane in drinking water disinfection by-product analysis. Presented at: 47th American Society for Mass Spectrometry Conference, Dallas, TX, June 13-17, 1999. — 6/13/1999

Contact: Paul H. Chen

Abstract: Tribromonitromethane (bromopicrin) has been found to be a disinfection by-product (DBP) in chlorinated1 and ozonated2 drinking water, and is structurally similar to dibromonitromethane, which has been indicated through structural analysis to be a possible carcinogen. Bromopicrin is thermally labile and decomposes at commonly applied GC injection port temperature (250?C).Thermolysis of bromopicrin generates ?CBr3, ?CBr2NO2, ?NO2, and Br? radicals which canundergo reactions with the solvent or combine with other radicals to form reaction products inthe GC injection port. Bromopicrin contains no hydrogen, but its mass spectrum shows peculiar[fragment + 1]+ ions for the fragment ions CBr2+, Br+, CBr+, and CNOBr+. The objectives of this investigation are (1) to identify the reaction products in several commonly used solvents, (2) to study the impact of thermal stability of bromopicrin and its decomposition products on drinking water analyses, and (3) to study the peculiar [fragment +1]+ ion phenomena.

Caughran, T.V., Richardson, S.D., Crumley, F.G., and Poiger, T. Does micro LC/MS offer advantages over conventional LC/MS in identifying disinfection by-products. Presented at: 47th American Society for Mass Spectrometry Conference, Dallas, TX, June 13-17, 1999. — 6/13/1999

Contact: Tashia V. Caughran

Abstract: Lower maximum contaminant levels (MCLs) of disinfection by-products were set for drinking water municipalities by the Stage 1 DBP Rule in November, 1998. With these new regulations, additional water treatment plants are expected to choose alternative disinfectants to chlorine. Although alternative disinfectants are gaining in popularity, not much is known about the by-products they produce. More research is needed to comprehensively identify these DBPs, and to determine what health effects these new DBPs have compared to those produced by chlorine. Many unidentified DBPs are believed to be in the polar fraction, which cannot be easily extracted from water. By using LC/MS instead of GC/MS, detection of these highly polar compounds should be possible, whereas GC/MS is not well suited for the determination of polar compounds. Micro LC/MS has become a popular technique for the analysis of complex pharmaceuticals, industrial chemicals, and other natural products. In those cases, it has offered lower detection levels (1). To our knowledge, the micro LC/MS technique has not been applied to the identification of drinking water disinfection by-products, which are typically present at low levels (ng/L-ug/L). In order to identify all possible polar DBPs in a drinking water mixture, our research group has conducted a study to determine whether the performance of a micro LC/MS system is superior to a conventional HPLC/MS system. In this study, a Fisons Platform quadrupole mass spectrometer was chosen as the detector, a Hewlett Packard 1050 HPLC system was used as the conventional HPLC, and a Microtech Ultra Plus system was chosen as the micro LC component. A series of standards, samples from drinking water plants in metropolitan Atlanta, and in Israel were analyzed. Other advantages and disadvantages of a micro LC/MS system over a conventional LC/MS system will be presented. The micro LC/MS system appears to produce a factor of 2x greater sensitivity compared to the conventional LC/MS system, and produced lower chemical background levels. However, reconstructed ion chromatograms are still necessary to observe the chromatographic peaks of the low-level DBPs.

	Presented	Published
Caughran, T.V., Richardson, S.D., Thruston, Jr., A.D., Chen, P.H., Collette, T.W., and Floyd, T.L. Identification of new drinking water disinfection by-products formed in the presence of bromide. Presented at: 217th American Chemical Society National Meeting, Anaheim, CA, March 21-25, 1999.	3/21/1999	
Contact: Tashia V. Caughran		
Abstract:		
Richardson, S.D., Caughran, T.V., Poiger, T., Guo, Y., and Crumley, F.G. Identification of polar drinking water disinfection by-products using LC/MS. Presented at: 217th American Chemical Society National Meeting, Anaheim, CA, March 21-25, 1999.	3/21/1999	
Contact: Susan D. Richardson		
Abstract:		
Richardson, S.D., Caughran, T.V., Guo, Y., Crumley, F.G., and Poiger, T. Identification of Polar Drinking Water Disinfection By-products with LC/MS. Abstract presented at: Georgia Water Resources Conference, Athens, GA, March 29-31, 1999.	3/29/1999	
Contact: Susan D. Richardson		
Abstract:		
Caughran, T.V., Richardson, S.D., Thruston, Jr., A.D., Chen, P.H., and Floyd, T.L. Are the newer, alternative disinfectants safer than chlorine for disinfecting drinking water?. Presented at: Georgia Water Resources Conference, Athens, GA, March 29-31, 1999.	3/29/1999	
Contact: Tashia V. Caughran		
Abstract:		
Caughran, T.V., Richardson, S.D., Thruston, Jr., A.D., Chen, P.H., Collette, T.W., and Floyd, T.L. Identification of New Drinking Water Disinfection By-products Formed in the Presence of Bromide. American Chemical Society, Anaheim, CA, March 21-24, 1999.	3/21/1999	
Contact: Tashia V. Caughran		
Abstract:		
Richardson, S.D., Caughran, T.V., Guo, Y., Crumley, F.G., and Poiger, T. Identification of polar drinking water disinfection By-products Using LC/MS. American Chemical Society, Anaheim, CA, March 21-24, 1999.	3/21/1999	
Contact: Susan D. Richardson		
Abstract:		
Kraemer, S.R., Johnston, J.M., and Colarullo, S.J. Investigation of Subsurface Residence Times in the Shallow Coastal Plain Aquifer Beneath Locust Grove, Maryland. ModelCARE'99, Zurich, Switzerland, September 20-23, 1999.	9/20/1999	
Contact: Stephen R. Kraemer		
Abstract:		

Jan 1, 1999 - Dec 31, 1999

Presented *Published*

Keyes, J.M.H., Frick, W.E., and Dufour, A.P. A case study using the EPA's water quality modeling system, the Windows Interface for Simulating Plumes (WISP). Presented at: 19th Annual American Geophysical Union Hydrology Days, Fort Collins, CO, August 16-20, 1999. — 8/16/1999

Contact: Walter E. Frick

Abstract: Wisp, the Windows Interface for Simulating Plumes, is designed to be an easy-to-use windows platform program for aquatic modeling. Wisp inherits many of its capabilities from its predecessor, the DOS-based PLUMES (Baumgartner, Frick, Roberts, 1994). These capabilities have been increased and improved. Wisp has been developed to supersede PLUMES upon its completion. To exemplify Wisp's capabilities, a case study is presented. This study is patterned after an existing facility but has been altered to demonstrate the interplay of various physical conditions. The purpose of presenting Wisp in this forum is to demonstrate its capabilities to the public and obtain feedback from potential users. A beta release is planned

Frick, W.E., and Keyes, J.M.H. Questioning the mach number criterion or why turbulent flow is compressible flow. Presented at: 19th Annual American Geophysical Union Hydrology Days, Fort Collins, CO, August 16-20, 1999. — 8/16/1999

Contact: Walter E. Frick

Abstract: According to Frick and Sigleo (1999) turbulence is a distinct and observable physical process in which flow, which is initially one-dimensional (the stem), is converted into two-dimensional radial flow (the cap) by shear. In the stem the incompressible equations of mass and momentum can be simultaneously satisfied. However, in the cap the flow is necessarily expansionary, causing a reduction in density and pressure. Since turbulence is therefore intrinsically compressible flow and since turbulent flow typically exists below the Mach number criterion for compressible flow, it is proposed that the commonly accepted Mach number criterion of 0.3 is much too high and that, in fact, the Reynolds number criterion for the onset of turbulent flow represents a better, if not the best, Mach number criterion. This work shows that compressible effects cannot be ignored in turbulent flow, i.e., for Mach number at least as low as 0.05.

Barnwell, Jr., T.O., and Levinson, B.M. U.S. Environmental Protection Agency's ecological research strategy. Presented at: International Congress on Ecosystem Health - Managing for Ecosystem Health, Sacramento, CA, August 15-20, 1999. — 8/15/1999

Contact: Thomas O. Barnwell

Abstract: EPA's Office of Research and Development (ORD) has recently released a research strategy to guide its program to improve ecosystem risk assessment and risk management, which is one of the Agency's higheset priority search areas (http://www.epa.gov/ORD/WebPubs/fmal/eco.pdf). It is ORD's vision that, in the next decade, EPA researchers will have developed the next generation of measurements, models and technologies necessary to protect both the present and probable fture sustainabidfty of ecosystems at local, watershed, and regional scales. The general direction of EPA's research program is to larger scales, a more holistic systems view, assessment of cumulative stress, determination of relative vulnerability to multiple stressors, and development of alternative management strategies for flexible decision-making. This research strategy supports EPA's changing regulatory perspective towards less centralized, more flexible decision-rnaking, and to more accountability to achieve results. Obviously, this is not a vision or goal that can be accomplished by ORD alone, but it is one that will be dependent on contributions from in-house and extramural research programs, other agencies, the academic community, states, and others. The purpose of this poster is to provide an overview of EPA's changing research program and discuss how the extramural community can contribute to it's success through the Science To Achieve Results (STAR) extramural research programs in Ecological Indicators, Regional Scaling, Water and Watersheds Research and Integrated Assessments.

Presented Published

Barnwell, Jr., T.O., and Levinson, B.M. U.S. Environmental Protection Agency's ecological research strategy. Presented at: Ecological Society of America Meeting, Spokane, WA, August 8-12, 1999. 8/8/1999

Contact: Thomas O. Barnwell

Abstract: In virtually every major environmental act, Congress has required that the U. S. Environmental Protection Agency (EPA) not only ensure that the air is safe to breathe, the water safe to drink, and the food supply free of contamination, but also that the environment is protected. As aresult, EPA's Office of Research and Development (ORD) has established research to improve ecosystem risk assessment and risk management as one of the highest priority research areas for investment over the next 10 years. The research is intended to provide environmental managers with new tools and flexible guidance that reflect a holistic environmental science and management perspective that can be applied both to common and unique problems. It is ORD's vision that, in the next decade, EPA researchers will have developed the next generation of measurements, models and technologies necessary to protect both the present and probable future sustainability of ecosystems at local, watershed, and regional scales. Obviously, this is not a vision or goal that can be accomplished by ORD alone, but it is one that will be dependent on contributions from in-house and extramural research programs, other agencies, the academic community, states, and others. The purpose of this poster is to provide an overview of EPA's changing research program and discuss how the extramural community can contribute to it's success.

Barnwell, Jr., T.O. North American Regional Action Plan on Mercury. Presented at: American Chemical Society, Anaheim, CA, March 21-24, 1999. 3/21/1999

Contact: Thomas O. Barnwell

Abstract: The North American Regional Action Plan (NARAP) on Mercury is one of a number of action plans that stem from the North American Agreement on Environmental Cooperation between the governments of Canada, Mexico and the United States. That Agreement established the Commission for Environmental Cooperation (CEC), which agreed to Resolution #95-5 on the Sound Management of Chemicals in 1995, which calls for the development of regional action plans for selected PBTs to address national and regional concerns. The objective of this action plan is to reduce anthropogenic sources of mercury through a program of capacity-building, pollution prevention and development of a cooperative scientific agenda. The NARAP also includes the expansion, to a North American scale, of some of the Canadian and US challenges contained in the Great Lakes Binational Toxics Strategy. The complete NARAP is available at www.cec.org.

BOOK CHAPTR

French, R.H., McCutcheon, S.C., and Martin, J.L. "Environmental hydraulics." In: Hydraulic Design Handbook, Chapter 5 L. Mays (Ed.), New York, NY: McGraw-Hill Professional 1999, 5.1-5.33. 7/29/1999

Contact: Steven C. Mccutcheon

Abstract: The thermal, chemical, and biological quality of water in rivers, lakes, reservoirs, and near coastal areas is inseparable from a consideration of hydraulic engineering principles: therefore, the term environmental hydraulics. In this chapter we discuss the basic principles of water and thermal budgets as well as mixing and dispersion.

JOURNAL

Zacharias, S., Heatwole, C.D., Persaud, N., Bruggeman, A.C., Kumar, D., and Smith, C.N. Stochastic simulation of field-scale pesticide transport using OPUS and GLEAMS. Journal of Environmental Quality 28 (2):411-423 (1999). 3/1/1999

Contact: Charles N. Smith

Abstract:

Smith, C.N., Payne, Jr., W.R., Pope, Jr., J.D., Winkie, J.H., and Parrish, R.S. A field study to compare performance of stainless steel research monitoring wells with existing on-farm drinking water wells in measuring pesticide and nitrate concentrations. Chemosphere 38 (4):875-889 (1999). 2/1/1999

Contact: Charles N. Smith

Abstract:

Presented *Published*

Molina, M., Araujo, R., and Hodson, R.E. Cross-induction of pyrene and phenanthrene in mycobacterium sp. isolated from polycyclic aromatic hydrocarbon contaminated river sediments. Canadian Journal of Microbiology 45 (6):520-529 (1999). 6/1/1999

Contact: Marirosa Molina

Abstract: A polycyclic aromatic hydrocarbon (PAH)-degrading culture enriched from contaminated river sediments and a Mycobacterium sp. isolated from the enrichment were tested to investigate the possible synergistic and antagonistic interactions affecting the degradation of pyrene in the presence of low molecular weight PAHs. The Mycobacterium sp. was able to mineralize 63% of the added pyrene when it was present as a sole source of carbon and energy. When the enrichment culture and the isolated bacterium were exposed to phenanthrene, de novo protein synthesis was not required for the rapid mineralization of pyrene, which reached 52% in chloramphenicol-treated cultures and 44% in the absence of the protein inhibitor. In the presence of chloramphenicol, <1% of the added pyrene was mineralized by the mixed culture after exposure to anthracene and naphthalene. These compounds did not inhibit pyrene utilization when present at the same time as pyrene. Concurrent mineralization of pyrene and phenanthrene after exposure to either compound was observed. Cross-acclimationbetween ring classes of PAHs may be a potentially important interaction influencing the biodegradation of aromatic compounds in contaminated environments.

Burke, Jr., R.A., Meyer, J.L., Cruse, J.M., Birkhead, K.M., and Paul, M.J. Soil-atmosphere exchange of methane in adjacent cultivated and floodplain forest soils. Journal of Geophysical Research 104 (D7):8161-8171 (1999). 4/1/1999

Contact: Roger A. Burke

Abstract:

Lewis, D.L. A sterilization standard for endoscopes and other difficult to clean medical devices. Practical Gastroenterology 23 (1):28-56 (1999). EPA/600/J-02/144. 10/15/1999

Contact: David L. Lewis

Abstract: An array of difficult to clean devices are used for diagnostic and surgical procedures involving various degrees of invasiveness. These range from prophylaxis angles used for cleaning and polishing teeth to flexible fiberoptic endoscopes for surgical procedures that penetrate the deepest recesses of the body. In 1992-93, the Food & Drug Administration (FDA) and the Centers for Disease Control and Prevention (CDC) adopted a sterilization standard for all reused dental devices entering the patient?s mouth. For endoscopy, however, they retained the same high-level disinfection standard deemed unsafe for dentistry. Federal agencies, therefore, haveestablished an enigmatic set of standards recommending sterilization of devices used to clean teeth, but not surgical devices that pass through the mouth and into the esophagus, lungs, and stomach.How uncertain is the science underpinning current infection control guidelines for endoscopy? To begin with, different federal agencies and professional organizations cannot agree on how long endoscopes should be soaked in a 2% glutaraldehyde solution, the most common germicide used on the devices. The system for reporting any resulting infections is equally unreliable. Even though endoscopes can infect patients with everything from virulent strains of enteric bacteria to sexually transmitted viruses, physicians usually have no way of knowing when it happens. The infected patients are diagnosed by their primary care physicians whoattribute their exposures to other risk factors.Most patients assume that endoscopes are sterilized and, if they ask their physicians, are usually told that they are. Because of long incubation times for many diseases, months or years may pass before infections aremanifested, thus diminishing the likelihood that they will be associated with endoscopic procedures. Even when occasional transmissions are suspected, it is unlikely that medical facilities or public health organizations will expend the substantial resources needed to carry out an investigation and document results in the medicalliterature. Despite this lack of documentation, data presented here conservatively indicate that 2.7% of the approximately 10 million procedures done each year in the U.S. with non-sterilized endoscopes cause infections. These 270,000 infections range in seriousness from subclinical to fatal. To provide patients with the widest margin of safety, endoscopes should meet certain minimum standards for cleanability and undergo an approved sterilization procedure after each use. Currently, the most practical approaches include automated reprocessing with liquid peracetic acid, which dissolves traces of patient materials, and sheathing the devicesso that patient-contaminated surfaces are discarded after each use.

Presented *Published*

Lewis, D.L., Garrison, A.W., Whittemore, A., Wommack, E., Steudler, P.A., and Melillo, J.M. Influence of environmental changes on degradation of chiral pollutants in soils. Nature 401 (6756):898-901 (1999). EPA/600/J-02/143. — 10/28/1999

Contact: David L. Lewis

Abstract: Numerous anthropogenic chemicals of environmental concern- including some phenoxy acid herbicides, organophosphorus insecticides, polychlorinated biphenyls, phthalates, freon substi- tutes and some DDT derivatives- are chiral. Their potential biological effects, such as toxicity, mutagenicity, carcinogenicity, and endocrine disrupter activity, are generally enantiomer- selective, and different enantiomers are preferentially degraded (transformed) by micro-organisms in various environments. Here we use field and laboratory experiments to demonstrate that environmental changes in soils can alter these preferences, and to suggest that the preferences shift owing to different groups of related microbial genotypes being activated by different environmental changes. In Brazilian soils, almost all pasture samples preferentially transformed the non-herbicidal enantiomer of dichlorprop ((RS)-2-(2,4-dichlorophenoxy)propionic acid), while most forest samples either transformed the herbicidal enantiomer more readily or as rapidly as the non-herbicidal enantiomer. Organic nutrient enrichments shifted enantioselectivity for methyl dichlorprop ((RS)-methyl 2-(2,4-dichlorophenoxy)propionic acid) strongly towards preferentially removing the non-herbicidal enantiomer in soils from Brazil and North America, potentially increasing phytotoxicity of its residues relative to that of the racemate. Assessments of the risks chemical pollutants pose to public health and the environment need to take into account the chiral selectivity of microbial transformation processes and their alteration by environmental changes, especially for pesticides as up to 25 per cent are chiral.

Kuhlbusch, T.A., and Zepp, R.G. Carbon trace gases in lake and beaver pond ice near Thompson, Manitoba, Canada. Journal of Geophysical Research 104 (D22):27693-27698 (1999). EPA/600/J-02/150. — 11/27/1999

Contact: Richard G. Zepp

Abstract: Concentrations of CO2, CO, and CH4 were measured in beaver pond and lake ice in April 1996 near Thompson, Manitoba to derive information on possible impacts of ice melting on corresponding atmospheric trace gas concentrations. CH4 concentrations in beaver pond and lake ice ranged between 0.3-150 mmol m(-3) and 3.1-56.2 mu mol m(-3), respectively. The corresponding CO concentrations showed no significant differences between the two lakes. They varied between 50 and 250 mu mol m(-3). These CO concentrations are some of the highest determined in any aquatic system. The differences in CH4 concentrations between lake and pond can be explained by the differences in production and microbial oxidation rates between the two systems. No explanation can be given for the similar CO concentrations. Supersaturation factors for CO were 660+/-130 and 630+/-330, and 65-35000 and 0.6-13 for CH4 in the ice of the beaver pond and Troy Lake, respectively. When digging into the beaver pond ice, a continuous flow of bubbles with 0.32+/-0.06 vol% CH4, 2.2+/-0.3 vol% CO2, and 482+/-98 ppb CO coming out of the slash ice for about 20-30 minutes was noticed. Wintertime flux estimates of CH4 and CO showed that they represent at minimum 6.4 % and 2.2 % of that of the summer. It has to be noted that these wintertime fluxes will mostly be released to the atmosphere during the time of snowmelt, thus a limited time period of weeks.

Smolen, J.M., Weber, E.J., and Tratnyek, P.G. Molecular probe techniques for the identification of reductants in sediments: evidence for reduction of 2-chloroacetophenone by hydride transfer. Environmental Science & Technology 33 (3):440-445 (1999). — 2/1/1999

Contact: Eric J. Weber

Abstract:

Susarla, S., Collette, T.W., Garrison, A.W., Wolfe, N.L., and McCutcheon, S.C. Perchlorate identification in fertilizers. Environmental Science & Technology 33 (19):3469-3472 (1999). — 10/1/1999

Contact: Steven C. Mccutcheon

Abstract: Perchlorate has contaminated groundwater, drinking water, and soils at several locations in the United States. The primary source of contamination at sites that have been investigated to date seems to be from industrial and military operations that use perchlorate as an oxidizing agent, However, recent examination of several fertilizers and fertilizer components showed that perchlorate is present at levels up to 0.84 wt %. These preliminary results suggest that fertilizers could be a source for perchlorate accumulation in the food chain.

Presented *Published*

Shevchenko, S.M., Bailey, G.W., and Akim, L.G. The conformational dynamics of humic polyanions in model organic and organo-mineral aggregates. Journal of Molecular Structure (Theochem) 460 (1-3):179-190 (1999). 2/26/1999

Contact: George W. Bailey

Abstract:

Sabaliunas, D., Ellington, J.J., and Sabaliuniene,I. Screening bioavailable hydrophobic toxicants in surface waters with semipermeable membrane devices: role of inherent oleic acid in toxicity evaluations. Ecotoxicology and Environmental Safety 44 (2):160-167 (1999). EPA/600/J-02/147. 10/19/1999

Contact: James J. Ellington

Abstract: Semipermeable membrane devices (SPMDs) were deployed for 4 weeks in two rivers in Lithuania, The SPMD dialysates were tested in the Microtox assay and, surprisingly, the sample from the relatively clean (U) over bar la River exhibited three times more toxicity than the sample from the Vilnia River receiving discharge from several industrial enterprises and municipal wastewater, The whole dialysates were subjected to bioassay-directed fractionation on silica gel columns. Toxicity testing of each fraction revealed that most of the toxicity was contained in fraction 10, which,vas eluted with 100% acetone. GC/FID, GC/ECD, and GC/FTIR/MS analysis of the fractions indicated that the major component of this fractionwas oleic acid. The oleic acid was most likely the hydrolysis product of methyl oleate, the major impurity of the SPMD triolein. It can be inferred that oleic acid was responsible for the toxicity of this fraction in Microtox, as a threefold difference in the toxicity between the two samples was also marked by a threefold difference in their oleic acid content. Toxicity of unsaturated fatty acids in various tests, including;Microtox, has been demonstrated elsewhere, Vilnia fraction 2, which was eluted with 100% hexane, exhibited the most toxicity of the remainder of silica gel fractions, The spectral analysis demonstrated that other toxic fractions contained a number of halogenated compounds and PAHs. In general, SPMDs have proved to be a useful way to screen for hydrophobic toxicants in water. However, sample clean-up procedures to remove oleic acid may be required prior to toxicity testing for the estimation of the true toxic potential of the accumulated pollutants.

Elovitz, M.S., and Weber, E.J. Sediment-mediated reduction of 2,4,6-trinitrotoluene and sorption of the resulting reaction products. Environmental Science & Technology 33 (15):2617-2625 (1999). EPA/600/J-99/238. 8/1/1999

Contact: Eric J. Weber

Abstract:

Ellington, J.J. Octanol/Water partition coefficients and water solubilities of phthalate esters. Journal of Chemical and Engineering Data 44 (6):1414-1418 (1999). EPA/600/J-02/146. 11/19/1999

Contact: James J. Ellington

Abstract: Measurements of the octanol/water partition coefficients (K-ow) and water solubilities of di-n-octyl phthalate (DnOP) and di-n-decyl phthalate (DnDP) by the slow-stirring method are reported. The water solubility was also measured for di-n-hexyl phthalate (DnHP). The log K-ow values of dimethyl phthalate (DMP), diethyl phthalate (DEP), di-n-butyl phthalate (DnBP), di-n-pentyl phthalate (DnPP), and DnHP, determined in a previous study, and the log K-ow values of DnOP determined again in this study were correlated against the number of carbons in the phthalate side chain. The straight line regression equation (log K-ow = 0.979 + 0.615, r(2) = 0.993) was used to extend the estimate for a carbon number 10; that is, log K-ow = 10.41 for DnDP. The slow-stirring log K-ow = 8.83 +/- 0.05 reported here for DnDP suggests that the decrease in solubility of the phthalate in the water layer is nonlinear when the side chain carbon length increases beyond eight carbons. Similarly, the straight line regression equation derived from correlation of the measured water solubilities for DnOP and DnHP reported here and the literature values for DMP, DEP, and DnBP against side chain carbon number predicted a 0.005 mu g/L water solubilty for DnDP. The measured water solubility of DnDP (0.22 +/- 0.05 mu g/L) reported here was 44-fold greater.

Susarla, S., Bacchus, S.T., Wolfe, N.L., and McCutcheon, S.C. Phytotransformation of Perchlorate and Identification of Metabolic Products in Myriophyllum aquaticum. International Journal of Phytoremediation 1 (1):97-107 (1999). EPA/600/J-02/141. 2/1/1999

Contact: Nelson L. Wolfe

Abstract:

Jan 1, 1999 - Dec 31, 1999

Presented Published

Bouchard, D.C. Sorption of vinclozolin and atrazine on four geosorbents. Pesticide Science 55 (11):1095-1102 (1999). EPA/600/J-02/142. 11/19/1999

Contact: Dermont Bouchard

Abstract: The objectives of this study were to evaluate the magnitude and kinetics of vinclozolin and atrazine sorption on one surface soil and three freshwater sediments using batch and column techniques. Data from miscible displacement column studies were analyzed using a two-domain, first-order mass transfer model to obtain the equilibrium sorption constant (K) and the first-order desorption rate coefficient (k2). In the two-domain conceptualization and mathematical model, sorption is assumed to be instantaneous (and therefore at equilibrium) in the first domain, and kinetically controlled (modeled as a first-order reaction) in the second domain. 3H2O used as a conservative tracer to characterize column hydrodynamics yielded breakthrough curves (BTCs) that were all symmetric and the data were described well by the advective-dispersive local equilibrium solute-transport model, thus indicating hydrodynamic equilibrium during transport for the column systems. However, vinclozolin and atrazine BTCs exhibited the tailing that is characteristic of non-equilibrium sorption during solute transport. The equilibrium model provided poor fits for all of the vinclozolin and atrazine data except for the least-sorbing geosorbent and atrazine where BTC symmetry was high. However, when slow sorption kinetics were accounted for, the two-domain model simulations provided good descriptions of the experimental data.

Ananyeva, N.D., Demkina, T.S., Jones, W.J., Cabrera, M.L., and Steen, W.C. Microbial biomass in soils of Russia under long-term management practices. Biology and Fertility of Soils 29 (3):291-299 (1999). EPA/600/J-02/149. 9/9/1999

Contact: William J. Jones

Abstract: Non-tilled and tilled plots on a spodosol (C-org 0.65-1.70%; pH 4.1-4.5) and a mollisol (C-org 3.02-3.13%, pH 4.9-5.3), located in the European region of Russia, were investigated to determine variances in soil microbial biomass and microbial community composition. Continuous, long-term management practices, including tillage and treatment with inorganic fertilizers or manure, were used on the spodosol (39 years) and mollisol (22 years). Total microbial biomass (C-mic), estimated by the substrate-induced respiration (SIR) method, and total fungal hyphae length (membrane filter technique) were determined seasonally over a 3-year period. Long-term soil management practices (primarily tillage and fertilizer application) led to decreases in total microbial biomass (80-85% lower in spodosol and 20-55% lower in mollisol), decreases in the contribution of C-mic to C-org (2.3- to 3.5-fold lower in spodosol and 1.2- to 2.3-fold lower in mollisol), and 50-87% decreases in total fungal hyphae length compared to non-tilled control plots. The contribution of fungi to total SIR in virgin mollisol and fallowspodosol plots was approximately 30%. However, the contribution of fungi to SIR was approximately two times greater in tilled spodosol plots compared to a fallow plot. In contrast, the contribution of fungi to SIR in tilled plots of mollisol was less (1.4-4.7 times) than for a virgin plot. In summary, long-term soil management practices such as tillage and treatment withorganic or inorganic fertilizers are important determinants of soil microbial biomass and the contribution of fungi to total SIR.

Tsiros, I.X., and Ambrose, Jr., R.B. An Environmental Simulation Model for Transport and Fate of Mercury in Small Rural Catchments. Chemosphere 39 (3):477-492 (1999). EPA/600/J-02/145. 8/1/1999

Contact: Robert B. Ambrose

Abstract:

Presented Published

Richardson, S.D., Thruston, Jr., A.D., Caughran, T.V., Chen, P.H., Collette, T.W., Floyd, T.L., Schenck, K.M., Lykins, Jr., B.W., Sun, G.R., and Majetich, G. Identification of new ozone disinfection by products in drinking water. Environmental Science & Technology 33 (19):3368-3377 (1999). 10/1/1999

Contact: Susan D. Richardson

Abstract: Using a combination of spectral identification techniques-gas chromatography coupled with low- and high-resolution electron-impact mass spectrometry (GC/EI-MS), low- and high-resolution chemical ionization mass spectrometry (GC/CI-MS), and infrared spectroscopy (GC/ IR)-we identified many drinking water disinfection byproducts (DBPs) formed by ozone and combinations of ozone with chlorine and chloramine. Many of these DBPs have not been previously reported. In addition to conventional XAD resin extraction, both pentafluorobenzyl-hydroxylamine (PFBHA) and methylation derivatizations were used to aid in identifying some of the more polar DBPs. Many of the byproducts identified were not present in spectral library databases. The vast majority of the ozone DBPs identified contained oxygen in their structures, with no halogenated DBPs observed except when chlorine or chloramine was applied as a secondary disinfectant. In comparing byproducts formed by secondary treatment of chlorine or chloramine, chloramine appeared to form the same types of halogenated DBPs as chlorine, but they were generally fewer in number and lower in concentration. Most of the halogenated DB Ps that were formed by ozone-chlorine and ozone-chloramine treatments were also observed in samples treated with chlorine or chloramine only. A few DBPs, however, were formed at higher levels in the ozone-chlorine and ozone-chloramine samples, indicating that thecombination of ozone and chlorine or chloramine is important in their formation. These DBPs included dichloroacetaldehyde and 1,1-dichloropropanone.

Richardson, S.D., Thruston, Jr., A.D., Caughran, T.V., Chen, P.H., Collette, T.W., Floyd, T.L., Schenck, K.M., Lykins, Jr., B.W., Sun, G.R., and Majetich, G. Identification of new drinking water disinfection byproducts formed in the presence of bromide. Environmental Science & Technology 33 (19):3378-3383 (1999). 10/1/1999

Contact: Susan D. Richardson

Abstract:

Richardson, S.D., Collette, T.W., Price, P.C., Genicola, F.A., Jenks, J.W., Thruston, Jr., A.D., and Ellington, J.J. Identification of drinking water contaminants in the course of a childhood cancer investigation in Toms River, New Jersey. Journal of Exposure Analysis and Environmental Epidemiology 9 (3):200-216 (1999). 7/1/1999

Contact: Susan D. Richardson

Abstract:

Richardson, S.D. Water analysis. Analytical Chemistry 71 (12):181R-215R (1999). EPA/600/J-02/148. 6/1/1999

Contact: Susan D. Richardson

Abstract: This review covers developments in water analysis from November 1996 to the end of October 1998, as found in the Chemical Abstracts Service CA Selects for gas chromatography, mass spectrometry, inorganic analytical chemistry, and pollution monitoring. In addition, because developments in the measurement of microorganisms is a fast-growing area, an effort was made to include up-to-date, important results as presented at the most recent Water Quality Technology Conference in November 1998. Microorganism studies have not appeared in previous Water Analysis reviews, but due to their increased importance, particularly with regard to outbreaks of illness from pathogenic organisms in drinking water and to new regulations for controlling them, they are included in this review. Also, in general, health effects studies are not covered in this review; however, a few significant ones are presented, as they relate to the ingestion of drinking water or to the toxicity of surface water. Numerous abstracts were consulted before choosing the best ones to present here. If an abstract was generally unclear or ambiguous, it was generally excluded. If the subject matter of the abstract appeared to be of a routine nature, with no new, significant findings, it was also generally excluded. For the most part criteria used for inclusion of a paper are in keeping with previous criteria used by former authors of prevous Water Analysis reviews. Further details of these criteria can be found in the 1991 Water Analysis review (Anal. Chem. 1991, 63, 301R-342R). Also, previous reviews of water analysis have focused mostly on methods development. This review contains not only important new methods but also important new findings or studies that were very comprehensive or particularly interesting. Because most water analysis publications involve environmental samples, this review was carefully coordinated with the Environmental Analysis review to minimize redundancies. In dividing the material to be covered, it was decided to cover drinking water entirely in this review, along with regulatory methods/regulations, microorganisms, general water quality/ nutrients, and QA/QC. Studies of pesticides and other pollutants in surface waters, groundwaters, seawaters, and wastewaters can be found in the Water Analysis Applications section of the Environmental Analysis review, also found in this issue of Analytical Chemistry.

RESEARCH RPT

Susarla, S., Bacchus, S.T., McCutcheon, S.C., and Wolfe, N.L. Potential species for phytoremediation of perchlorate. Athens, GA: US Environmental Protection Agency. 1999. EPA/600/R-99/069 (NTIS PB2000-102483). 8/15/1999

Contact: Steven C. Mccutcheon

Abstract: Phytoremediation is the use of plants to cleanse soil and water contaminated with organic or inorganic pollutants. This promising new field of research can be used for in situ clean up of large volumes and expansive areas of contaminated soils or waters, including ground water. Three laboratory-scale experiments were conducted to: 1)evaluate the ability of selected terrestrial, wetland, and aquatic plants to remove perchlorate from an aqueous solution; 2)compare the performance of different age classes of one plant species; 3)evaluate the role of nutrients on perchlorate removal; 4)determine the fate of perchlorate removed from solution (e.g., plant tissue distribution; accumulation vs. breakdown); 5)document external plant responses to perchlorate; and 6)predict field-scale performance of the plant species evaluated. Perchlorate concentrations of 0.2, 2.0, and 20 ppm were tested in aqueous and sand treatments for ten-day periods in each experiment.